

**SIMULATION OPTIMIZATION UNDER INPUT UNCERTAINTY:  
FORMULATIONS, ALGORITHMS, AND INSIGHTS**

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By

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## SUMMARY

Simulation optimization is concerned with identifying the best design for large, complex and stochastic physical systems via computer simulation models. Its applications span across various fields including transportation, finance, power, healthcare, etc. In building a stochastic simulation model, one often needs to specify a set of distributions, known as “input distributions”. However, since these distributions are usually estimated using finite real-world data, the simulation output is subject to the so-called “input uncertainty”. Existing studies indicate that ignoring input uncertainty can cause a higher risk of selecting an inferior design in simulation optimization. This thesis is therefore devoted to addressing input uncertainty in the context of simulation optimization by proposing new formulations, devising new algorithms, and developing insights for improving existing algorithms.

In Chapter 2, we study a simulation optimization problem with a general design space. The scenario of interest is when a set of fixed input data is given and no additional data is available. To hedge against the risk of input uncertainty, we propose a Bayesian Risk Optimization (BRO) framework that (i) models input uncertainty using posterior distributions; (ii) incorporate a decision maker’s risk preference via risk measures such as value-at-risk (VaR) and conditional value-at-risk (CVaR). We establish the asymptotic properties of BRO, and reveal that BRO essentially seeks a balance between predicted average performance and the uncertainty in a design’s actual performance.

Chapter 3 considers optimizing over a finite design space, a problem known as Ranking and Selection (R&S) in statistics literature, or Best-Arm Identification in Multi-Armed Bandits literature. We look closely into the classical fixed budget R&S without input uncertainty, which will be a fundamental building block of Chapter 4 for studying R&S under input uncertainty. Specifically, we investigate the performance of a widely used algorithm called Optimal Computing Budget Allocation (OCBA). Our analysis leads to a surprising insight: the popular implementation of OCBA suffers from a slow convergence rate. We

then propose a modification to boost its performance, where the improvement is shown by a theoretical bound and numerical results. In addition, we explicitly characterize the convergence rate of several simplified algorithms, showcasing some interesting findings as well as useful techniques for convergence analysis.

In Chapter 4, we study R&S under input uncertainty where additional data can be acquired to reduce input uncertainty. To the best of our knowledge, this setting has rarely been studied in existing literature. Two classical formulations of R&S, i.e., fixed confidence and fixed budget, are extended to our new settings. New algorithms are developed to (i) achieve a statistical selection guarantee when new data arrive sequentially; (ii) efficiently allocate a finite budget between data collection and simulation experimentation. Theoretical guarantees are provided for our algorithms, and numerical results demonstrate their effectiveness.

# CHAPTER 1

## INTRODUCTION

Stochastic simulation is a powerful tool for modeling large-scale complex real-world systems arising in transportation, finance, power and many other fields. Using simulation to identify the best system design is generally referred to as simulation optimization or Optimization via Simulation. A sharp advantage of simulation-based approaches is the low cost of computer experiments compared with expensive physical experiments. For instance, a carefully built simulation model may enable an aircraft engine manufacturer to select the optimal engine design without suffering the potential high loss from a disastrous failure in field experiments.

In practice, the success of simulation optimization hinges on a number of key factors, and a practitioner is frequently faced with the following challenges.

1. *Model logic discrepancy*. Sometimes a simulation model does not faithfully represent the underlying deterministic logic of the physical system being modeled, which can be physical laws (e.g., aerodynamics) or man-made rules (e.g., traffic rules). This inconsistency will result in a systematic error in simulation output.
2. *Input uncertainty (IU)*. To capture the uncertainty in real-world systems (e.g., weather condition, traveling time, etc.), a set of probability distributions are often estimated from finite real-world data. These distributions, known as “input distributions”, are then specified as part of the input to the simulation model, causing error that propagates to simulation output.
3. *Simulation uncertainty (SU)*. This refers to the error caused by using finite simulation runs (or finite amount of simulation time) to estimate a design’s performance. For

example, the expected cost under an inventory policy is estimated by averaging over a finite number of simulation outputs, and is thus subject to finite-sample error.

4. *Algorithm efficiency.* Last but not least, the efficiency of optimization algorithm is critical to finding an optimal or near-optimal design. However, in contrast to classical stochastic optimization, objective function evaluation in simulation optimization is noisy and time-consuming, and there may be little structure to exploit.

Among the aforementioned challenges, although model logic misspecification is of great practical interest to study, the related analysis is typically application-specific and a general quantitative framework is still lacking. Therefore, the focus of this thesis is on challenges 2,3 and 4. In particular, we study simulation optimization under IU, which has not been studied extensively in the literature despite its well-recognized importance. As a high-level overview, we approach this problem in three aspects.

First, we consider a simulation optimization problem with general design space, where the input dataset is given and fixed. A Bayesian Risk Optimization (BRO) framework is proposed to hedge against the risk associated with IU. We establish the asymptotic properties of BRO, and further reveal that BRO is able to achieve a balance between predicted average performance and the risk in a design’s actual performance.

Then, we study simulation optimization over a finite design space, a problem known as Ranking and Selection (R&S). We delve into the classical fixed budget R&S without IU, since it is an essential building block for studying R&S under IU. Specifically, we investigate a widely used and studied algorithm called Optimal Computing Budget Allocation, and show that its popular implementation actually suffers from a slow convergence rate. A modification is then proposed to provably improve its performance. Furthermore, we explicitly characterize the convergence rate of several simplified algorithms to shed some light on existing algorithms’ properties, while developing useful techniques for conducting general convergence analysis in fixed budget R&S.

Finally, we study R&S under IU, where additional data can be acquired to reduce IU. To the best of our knowledge, this setting has seldom been studied in existing literature. We extend two classical R&S formulations, i.e., fixed confidence and fixed budget, to account for the mixed impact of IU and SU. New algorithms are developed to solve the formulated problems, with theoretical guarantees provided on their performance. The effectiveness of our algorithms is also demonstrated numerically.

## 1.1 General Simulation Optimization under Input Uncertainty

### 1.1.1 Background and Motivation

In many simulation optimization problems, the objective function is in the form of an expectation taken with respect to some underlying distribution. For example, a classical newsvendor problem involves maximizing the expected profit by choosing an optimal order quantity, where the expectation is taken with respect to the demand distribution. Such distributions are specified as an input to the simulation model, hence the name “input distributions”. Traditionally, the study of simulation optimization assumes full knowledge of the input distributions, and the primary focus is on tackling the uncertainty within the simulation model, i.e., simulation uncertainty (SU).

In practice, input distributions are often estimated from a finite amount of input data, so the resulting model is also subject to input uncertainty (IU). However, in contrast to SU, which can be reduced by increasing simulation effort, IU may be uncontrollable due to the difficulty in acquiring additional input data. Consequently, if we optimize a model which is built on input distributions estimated from a small number of data samples, the obtained optimal design may have a poor performance under the true input distribution. To see the risk of ignoring IU, consider a newsvendor problem with lost sales, where the goal is to maximize the expected profit under stochastic demand. Suppose that the demand is exponentially distributed with rate  $\theta^c = 1/20$ , and the unit price and unit cost are 2 and 1, respectively. We draw 1,000 sets of independent and identically distributed (i.i.d.)

demand data, each dataset of size 20. Then, for each dataset we compute a maximum likelihood estimate of  $\theta^c$ , which is plugged into the model to solve an approximate problem. The histograms of the resulting optimal designs and their corresponding true performances (under  $\theta^c$ ) are shown in figure 1.1. Although the average optimal design is close to the true optimal design 13.8629, the extreme values could reach 5 and 25. Similarly, the extreme performance of designs can be as low as 3 compared with the true optimal performance 6.1371. In other words, the decision maker may suffer a great loss if s/he blindly assumes that the estimated input distribution is accurate. This example illustrates the importance of accounting for IU in simulation optimization.

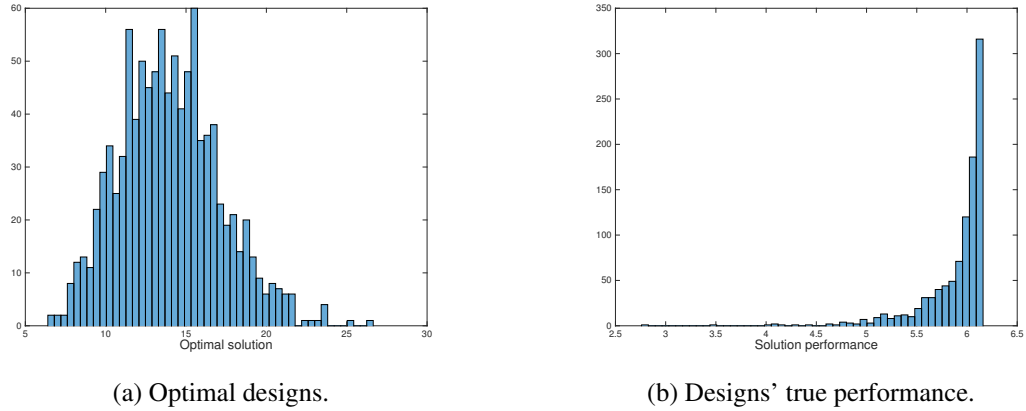


Figure 1.1: Input uncertainty in a newsvendor problem.

### 1.1.2 Literature Review

There is a rich body of literature on quantifying the mixed impact of IU and SU on simulation output. The methods proposed so far in the literature can be roughly grouped into two major categories. One is the frequentist methods that allow nonparametric input distributions and use direct or bootstrap resampling techniques to assess IU (e.g., [1, 2, 3]). The other is the Bayesian model averaging methods (e.g., [4, 5, 6]) that assume a parametric model and use the posterior distribution of unknown parameters as the sampling distribution during simulation process. In addition to these methods, [3] used delta method

to decompose the variance of simulation output into two parts corresponding to SU and IU. [7] proposed a method for quickly assessing the relative contribution of each input distribution to the overall effect of IU. [8] quantified the risk of IU via their proposed efficient estimators based on nested simulation. Recent advances in stochastic kriging [9] also gives rise to the application of meta-model assisted method in quantifying IU (see, e.g., [10, 11, 12]).

Simulation optimization under IU, on the other hand, has not been studied as extensively. Some recent research touches upon the case of a finite design space, but we defer the review on this line of works to Section 1.3.2. In many applications, finding designs with an acceptable level of potential risk is at least as important as achieving good average performance. For example, in the aforementioned newsvendor problem with IU, a risk-averse manager would base the order quantity on both the estimated expected profit and the risk of a large loss. In other cases, such as the operation of hospital emergency rooms and massive electric power systems, there is even a greater need for controlling the risk of extreme performance because the failure of these systems, no matter how unlikely it may seem, can result in catastrophic consequences.

Since we are concerned about the extreme performance caused by IU, perhaps the most relevant approach is distributionally robust optimization (DRO). The idea of DRO is to optimize the worst-case performance over a family of possible input distributions. An abundant literature exists on DRO and we refer the reader to [13, 14, 15, 16] for reviews and recent development. The key to DRO is to construct a reasonable uncertainty/ambiguity set that allows computational tractability while maintaining certain performance guarantees. Two typical ways to construct the uncertainty set are based on: (i) distance metrics, such as  $\phi$ -divergence and Wasserstein distance (see e.g. [17, 18, 19, 15, 20]); (ii) moment constraints (see e.g. [21, 16, 22, 23]). Nonetheless, DRO's reliance on the uncertainty set have mixed outcomes: as was observed in [24], an inappropriately constructed uncertainty set may produce excessively conservative designs, i.e., designs that perform poorly under



far more realistic scenarios than the worst case.

In light of the aforementioned drawback of DRO, we propose a Bayesian Risk Optimization framework as an alternative approach. More specifically, we formulate a new optimization problem and investigate its asymptotic properties, which is closely related to existing studies on the statistical properties of stochastic programs. For example, [25] discussed a general approach to studying the asymptotics of statistical estimators in stochastic programming, and [26] investigated the asymptotic properties of optimal values and solutions for the sample average approximation problem. Notably, [27] also established central limit theorems for composite risk functionals, and discusses the asymptotic behavior of stochastic programs with objectives being composite risk functionals. Nevertheless, aside from the difference in settings (frequentist vs. Bayesian), the major distinction between [27] and our work lies in the distributions to which risk functionals are applied and the associated proof techniques. On the one hand, [27] considered a class of risk functionals applied to a sequence of empirical distributions, where a version of uniform Central Limit Theorem and an extended Delta Theorem can be applied to show the weak convergence of risk functionals. On the other hand, we apply risk functionals to a sequence of posterior distributions, where a Bayesian Central Limit Theorem guarantees that the total variation distance between the posterior distribution and a normal distribution (with a random mean) vanishes in probability. The theorem’s intricate form adds more technicalities and subtleties to our analysis. In particular, a given risk functional is not necessarily uniformly continuous relative to the total variation metric. In addition, while [27] studied the asymptotic properties of risk functional as an estimator of a “true” functional, we study similar asymptotics in an effort to uncover the implications of solving our proposed optimization problem.

### 1.1.3 Main Contributions

To explore the middle ground between optimistically ignoring IU and pessimistically fixating on the worst case, we propose a Bayesian Risk Optimization (BRO) framework. BRO differs from DRO in two aspects. First, it takes a Bayesian perspective and characterizes the degree of IU through a posterior distribution instead of an uncertainty set. Second, BRO allows a risk measure to be applied, which incorporates a range of risk preferences beyond optimizing over the worst case.

The BRO framework first appeared in a preliminary work [28], in which four choices of risk measures were considered: mean, mean-variance, value-at-risk (VaR) and conditional value-at-risk (CVaR). Despite the possible benefits suggested by numerical evidence, it is not clear what kind of “robustness” can be gained from considering the BRO formulations. To develop a deeper understanding of BRO, we make the following contributions.

1. Focusing on the aforementioned four choices of risk measures, we establish the consistency of objective functions and optimal designs, as well as the asymptotic normality of objective functions and optimal values.
2. More importantly, our analysis reveals a hidden interpretation: *the objectives of BRO can be approximately viewed as a weighted sum of posterior mean objective and the (squared) half-width of the true objective’s confidence interval.*

Interestingly, similar insight has also been developed for DRO in [29], which showed that a large class of robust empirical optimization problems are essentially equivalent to a mean-variance formulation. In the same spirit, [30] showed that the robust sensitivity of an expectation with respect to the unknown distribution can be decomposed as the mean plus a term which depends on the standard deviation. Nevertheless, due to the fundamental differences between DRO and BRO, a direct comparison between these two formulations is difficult, if not impossible. Instead, our work aims to provide a different approach to IU, which hopefully will add one more option to the toolbox of practitioners.

## 1.2 Classical Fixed Budget Ranking and Selection

### 1.2.1 Background and Motivation

Simulation optimization over a finite design space is also known as Ranking and Selection (R&S) in statistics literature, or Best-Arm Identification in Multi-Armed Bandits literature. In this part, we study the classical fixed budget formulation of R&S, where IU does not exist and the main difficulty stems from SU. Aside from being of independent interest to study, this problem could also serve as a fundamental building block for studying R&S under IU. As we shall see in Chapter 4, the second stage problem in the proposed new fixed budget formulation exactly reduces to classical fixed budget R&S.

In fixed budget R&S without IU, the main challenge is in how to make the best use of a finite simulation budget (computational resource) to efficiently select the best design. On the one hand, a design’s performance needs to be estimated via Monte Carlo simulation, which requires multiple simulation runs/replications. On the other hand, each simulation run can be time-consuming for sophisticated simulation models. Numerous algorithms have been proposed for budget allocation, among which the Optimal Computing Budget Allocation (OCBA) algorithm is arguably one of the most widely used and studied. However, despite the abundant empirical evidence on OCBA’s robust performance, a major criticism is that no theoretical guarantee has been provided to this date. This motivates us to develop a deeper understanding of OCBA, as it can also help us gain useful insights for improving existing algorithms as well as designing new algorithms.

### 1.2.2 Literature Review

The research on R&S is largely concerned with two related yet distinct formulations. The fixed confidence formulation aims to attain a target confidence level of the selected design’s quality using as little simulation effort as possible, whereas the fixed budget formulation typically requires maximizing the probability of correct selection (PCS) under a fixed bud-

get of simulation runs. For fixed confidence, a considerable amount of research effort goes to the indifference zone (IZ) formulation, which dates back at least to [31]. An IZ procedure allows the user to specify the smallest difference in performance worth detecting, and it guarantees selecting the best design with (frequentist) probability higher than a prespecified level (e.g., 95%), provided that the difference between the top-two designs is sufficiently large. Numerous efficient IZ procedures have been proposed in simulation literature, including but are not limited to the KN procedure in [32], the KVP and UVP procedures in [33], and the BIZ procedure in [34]. We refer the reader to [35] and [36] for excellent reviews of the development on this topic. In addition, the Bayesian approaches (see, e.g., [37]) and the probably approximately correct (PAC) selection (see, e.g., [38]) have also been studied in this stream of works.

In this part of the thesis, we study the fixed budget formulation under a frequentist setting. In simulation optimization, the Optimal Computing Budget Allocation (OCBA) algorithm in [39] has been widely used and studied. Although OCBA is usually derived under a normality assumption and asymptotic approximations, it is well known for its robust empirical performance even when the sample distributions are non-normal. Moreover, its key allocation rule can be formally justified from the perspective of the large deviations theory (see, e.g., [40]). However, a major criticism is that a theoretical performance guarantee is still lacking to this date, mostly due to the difficulties in characterizing the PCS for sequential sampling algorithms. On the other hand, in the Multi-Armed Bandit literature, the same problem has been studied under the name of “Best-Arm Identification”, where the Successive Rejects (SR) algorithm proposed in [41] currently stands as one of the best algorithms. Built on a framework of sequential elimination, SR not only achieves good performance but also allows a finite-sample bound to be derived. Furthermore, [42] showed that SR can match the optimal rate up to some constant in the Bernoulli setting. Nevertheless, SR’s performance under general distributions has not yet been studied. Bayesian methods are also gaining momentum recently. For example, the simple Bayesian algorithms proposed

in [43] were shown to achieve the optimal posterior convergence rate. However, there was no guarantee on the frequentist performance. The follow-up work, [44], improved the Expected Improvement method and provided a frequentist bound, but the guarantee was for the fixed confidence setting.

Among the aforementioned algorithms, OCBA has the most variants and extensions. It has been extended to multi-objective optimization ([45]), finding simplest good designs ([46]), R&S under input uncertainty ([47]), optimizing expected opportunity cost ([48]) and many others. Meanwhile, attempts have been made to approach the problem from different perspectives. For example, [49] considered fixed budget R&S under a Bayesian framework and formulated the problem as a Markov Decision Process, allowing a Bellman equation and an approximately optimal allocation to be derived. Also interestingly, [50] revealed that some variants of the Expected Improvement methods essentially have the same allocation as the OCBA methodology. Nonetheless, as was mentioned in [51] as one of the open challenges, “there is no theoretical proof to show how good the finite-time performance of OCBA is with respect to the real problem”.

### 1.2.3 Main Contributions

The purpose of our research is to better understand existing algorithms’ behavior through rigorous analysis, and develop insights for improving their performance. In particular, our work highlights convergence analysis on the OCBA algorithm and some of its variants, where the convergence rate is measured in terms of the large deviations rate of the probability of false selection (PFS). Specifically, our contributions are summarized as follows.

1. We show that for three OCBA-type algorithms including the original OCBA, a budget-independent initial sample size only amounts to a sub-exponential (or even polynomial) convergence rate of the PFS.
2. By making the initial sample size increase linearly with the total budget, we improve

the convergence rate to exponential, as is shown by a finite-sample bound on the PFS. The improvement is further validated via numerical experiments.

3. As further exploration towards general convergence analysis, we exactly characterize the convergence rate of two simplified algorithms for a two-design case, where the results showcase some interesting insights as well as useful proof techniques.

### **1.3 Ranking and Selection under Input Uncertainty**

#### 1.3.1 Background and Motivation

In the presence of IU, an R&S algorithm may end up selecting an inferior design even using infinite simulation effort. Although IU can only be reduced by collecting more data, most studies assume that the input dataset is *given and fixed*, because acquiring additional data can be expensive and time-consuming (e.g., collecting medical data by running clinical trials). However, there are also cases where new data can be accessed at a reasonable pace and cost. For instance, an online retailer gets to observe the demand of a certain product every week. Similarly, a wind power plant has built-in sensors that gather wind data on a daily basis. In these scenarios, a moderate amount of data can be collected periodically, and it motivates us to extend existing R&S formulations so that IU and SU can be controlled within a unified decision-theoretic framework.

#### 1.3.2 Literature Review

As was pointed out in [52], directly applying classical R&S algorithms by ignoring IU can be misleading and may render selection guarantee invalid. In light of such observations, recent effort has been made to account for IU when the input dataset is given and fixed. For instance, in the fixed confidence setting, [53] took a Bayesian perspective and selected the design with the best performance averaged over the posterior distribution of input models; [52] and [54] considered a fixed confidence formulation under an IZ setting, and both dis-

covered that a larger IZ parameter is required to maintain the desired statistical guarantee under IU; [55] took a distributionally robust approach by comparing the designs based on their worst-case performance over a finite set of possible input distributions. In the fixed budget setting, [47] seems to be the only work in this category, and they combined a distributionally robust perspective with the OCBA framework. Aside from selection algorithms, [56] proposed a comparison algorithm which exploits the common input distribution effect to construct simultaneous confidence intervals for all designs' performance. However, despite these efforts devoted to R&S under IU, the possibility of collecting additional data is often not taken into consideration.

In our work, we consider the optimal joint decision of data acquisition and simulation experimentation. The most relevant work in this regard is [57], which studied how to balance input data size and simulation effort to minimize the asymptotic variance of a *single design's* performance estimator. However, to the best of our knowledge, we are among the first to consider such tradeoff in an optimization (R&S) context. In addition, our fixed budget setting is somewhat related to [58], in which the authors weighed the benefit of running simulations against the opportunity cost of delay in decision making, but their setting did not have IU as a concern.

### 1.3.3 Main Contributions

We consider the following two settings where additional input data can be collected to reduce IU.

- (i) *Fixed confidence.* Suppose that data become available in an online fashion, e.g., new data arrive sequentially over time. For the purpose of R&S, the new data can be used to refine our input distribution estimates, and additional simulations can be run to improve the estimates of the designs' performance. Then, the question is how to leverage the incoming data to identify the best design with, e.g., 95% probability, as quickly as possible. A hidden challenge here is how to aggregate simulation outputs

that are generated under different input distributions.

- (ii) *Fixed budget.* Suppose that a certain form of budget is given, which can be used to collect input data as well as run simulations. The goal is to maximize the probability of correct selection by striking a balance between data acquisition and simulation experimentation. A natural case is when both costs are measured in time units, so long as they are on comparable scales. The budget could also be measured in terms of monetary value, since some data can be purchased from data vendors (e.g., financial transaction data), and simulations can be run on commercial cloud computing platforms, which is usually priced based on running time and the types of machines used.

The above settings essentially raise two central questions. First, what can we do if we can acquire more data? Second, how much data is “enough”? These questions are addressed through the following contributions.

1. In the fixed confidence setting, we extend and modify a Sequential Elimination framework to allow pairwise comparisons, which significantly improves selection efficiency compared with directly extending the Sequential Elimination framework. We provide upper bounds on the expected running time required for our algorithm to terminate, and propose a heuristic method to further boost efficiency.
2. In the fixed budget setting, we propose an algorithm, OCBAIU, which can effectively balance IU and SU, and achieve a near-optimal probability of correct selection for different configurations of problem instances and cost parameters. A finite-sample bound is also provided on the probability of false selection.
3. In designing the aforementioned algorithms, we establish a few asymptotic normality results for online as well as nested estimators, which are of independent interest. Our result on an online estimator explicitly characterizes the bias-variance tradeoff in



aggregating simulation outputs under repeatedly updated input distributions. Meanwhile, our result for the nested estimator closely mirrors a classical result in [3] on decomposing the variance caused by IU and SU.

4. Finally, we demonstrate the effectiveness of our algorithms on a production-inventory problem. The numerical results suggest that the proposed methods work well for both single input distribution (one source of IU) and multiple input distributions (four independent sources of IU).

## 1.4 Thesis Outline

The rest of the thesis is organized as follows. In Chapter 2, we formally introduce the BRO framework, establish some related asymptotic properties, and reveal the hidden implication of solving a BRO problem. Chapter 3 pushes the boundary of classical fixed budget R&S by investigating the convergence rate of OCBA and some simplified algorithms. The obtained insights have proven useful for improving existing algorithms both theoretically and practically. Chapter 4 studies R&S under IU where additional data can be collected. We extend two classical formulations to our settings, and develop algorithms to solve the new formulations.

We also note that the notations used in each chapter will be self-contained. In other words, any notational overlap should cause no confusion, since each chapter is independent of the others. By redefining some notations as necessary, we avoid introducing an overly complicated system of notations.

## CHAPTER 2

### A BAYESIAN RISK APPROACH TO SIMULATION OPTIMIZATION UNDER INPUT UNCERTAINTY: FORMULATIONS AND ASYMPTOTICS

In this chapter, we propose a Bayesian Risk Optimization approach to addressing input uncertainty in simulation optimization. Through asymptotic analysis, we reveal a hidden interpretation of the formulated optimization problems.

The rest of this chapter is organized as follows. In Section 2.1, we review some necessary preliminaries and formally introduce the Bayesian Risk Optimization framework. Sections 2.2 and 2.3 establish a series of consistency and asymptotic normality results for the proposed optimization problem. Section 2.4 discusses the hidden interpretation of solving a Bayesian Risk Optimization problem. Concluding remarks are made in Section 2.5.

#### 2.1 Preliminaries

##### 2.1.1 Basic Setup

We consider the following general simulation optimization problem,

$$\min_{x \in \mathcal{X}} \mathbb{E}_{\mathbb{P}^c}[h(x, \xi)], \quad (2.1.1)$$

where  $\mathcal{X}$  is a closed subset of  $\mathbb{R}^d$  representing the design space,  $\xi$  is a random vector in  $\mathbb{R}^m$  capturing the system's intrinsic uncertainty, and  $h$  is a system performance measure function that maps  $\mathbb{R}^d \times \mathbb{R}^m$  to  $\mathbb{R}$ . The expectation  $\mathbb{E}$  is taken with respect to (w.r.t.) the distribution of  $\xi$ , denoted by  $\mathbb{P}^c$ . Since (2.1.1) is also a generic stochastic optimization problem, we will refer to a design  $x \in \mathcal{X}$  as a solution, and the expected performance of  $x$  as the objective function.

Although (2.1.1) formulates a broad range of decision-making problems, it seems to

overlook the fact that  $\mathbb{P}^c$  is rarely known exactly in practice. More likely is that only an estimate  $\hat{\mathbb{P}}$  can be obtained using finite real-world input data. However, due to finite-sample error, even if the approximate problem

$$\min_{x \in \mathcal{X}} \mathbb{E}_{\hat{\mathbb{P}}} [h(x, \xi)] \quad (2.1.2)$$

is solved to optimality, the resulting solution may not perform quite as well under the true distribution  $\mathbb{P}^c$ . The estimation error in  $\hat{\mathbb{P}}$  is commonly referred to as input uncertainty (IU) in simulation optimization, or distributional uncertainty in stochastic optimization. One popular approach to addressing IU is to apply the framework of distributionally robust optimization (DRO), where one uses available data to construct an uncertainty/ambiguity set  $\mathcal{D}$  that contains  $\mathbb{P}^c$  with a high probability, and then optimize over  $\mathcal{D}$  by hedging against the worst case, i.e.,

$$\min_{x \in \mathcal{X}} \max_{\mathbb{P} \in \mathcal{D}} \mathbb{E}_{\mathbb{P}} [h(x, \xi)]. \quad (2.1.3)$$

As is mentioned in [59], the idea of robust optimization in stochastic programming dates back at least to [60], and one can refer to [61] for a thorough discussion. The key to the success of DRO is to construct a reasonable  $\mathcal{D}$  such that (2.1.3) is computationally tractable while maintaining certain performance guarantees. However, DRO's reliance on  $\mathcal{D}$  can be a double-edged sword: as is observed in [24], an inappropriately constructed  $\mathcal{D}$  may lead to overly conservative solutions, i.e., solutions that perform poorly under far more realistic scenarios than the worst case.

### 2.1.2 Construction of Probability Space

We consider a case where  $\mathbb{P}^c$ , i.e., the true underlying distribution of  $\xi$  in (2.1.1), belongs to a parametric family of distributions  $\{\mathbb{P}_{\theta} \mid \theta \in \Theta\}$ , where  $\Theta$  is the parameter space. In particular, this encompasses distributions with a finite support, where the probability mass vector can be treated as a finite-dimensional parameter. Suppose that the form of  $\mathbb{P}_{\theta}$  is

known but the true parameter  $\theta^c$  is not. Through a Bayesian perspective, we view  $\theta^c$  as a realization of a belief random variable  $\tilde{\theta}$ . Denote by  $\pi$  the prior distribution of  $\tilde{\theta}$ . Also assume that we have a dataset  $\{\xi_i\}_{i=1}^n$ , which, conditioned on  $\tilde{\theta}$ , are  $n$  independent and identically distributed (i.i.d.) samples with distribution  $\mathbb{P}_{\tilde{\theta}}$ . To perform a rigorous analysis of BRO's asymptotic properties, we explicitly construct a probability space  $(\Omega, \mathcal{F}, \mu)$  such that (i) both  $\tilde{\theta}$  and  $\xi_i$  are random variables defined on this space; (ii)  $\tilde{\theta}$  follows the prior distribution  $\pi$ ; (iii) conditioned on  $\tilde{\theta}$ ,  $\{\xi_i\}$  are i.i.d. samples from  $\mathbb{P}_{\tilde{\theta}}$ . Our construction follows the standard approach in Bayesian literature (e.g., [62]).

Suppose that  $\tilde{\theta}$  takes value in a parameter space  $\Theta \subset \mathbb{R}^l$  equipped with a Borel  $\sigma$ -algebra  $\mathcal{B}_\Theta$  and a probability measure  $\pi$ , while  $\xi_i$  takes value in  $\Xi \subset \mathbb{R}^m$  equipped with a Borel  $\sigma$ -algebra  $\mathcal{B}_\Xi$  and a collection of probability measures  $\{\mathbb{P}_\theta\}_{\theta \in \Theta}$ . Then, the probability space induced by  $n$  i.i.d. copies of  $\xi_i$  is  $(\Xi^n, \mathcal{B}_\Xi^n, \mathbb{P}_\theta^n)$ , where  $\mathcal{B}_\Xi^n$  is the product  $\sigma$ -algebra  $\mathcal{B}_\Xi \otimes \cdots \otimes \mathcal{B}_\Xi$ <sup>1</sup> and  $\mathbb{P}_\theta^n$  is the product measure  $\mathbb{P}_\theta \times \cdots \times \mathbb{P}_\theta$ . Next, we apply Kolmogorov's Extension Theorem (see, e.g., [63, Theorem A.3.1]) to extend  $(\Xi^n, \mathcal{B}_\Xi^n, \mathbb{P}_\theta^n)$  to a sequence space  $(\Xi^\mathbb{N}, \mathcal{B}_\Xi^\mathbb{N}, \mathbb{P}_\theta^\mathbb{N})$ , where  $\Xi^\mathbb{N}$  is the space of all infinite sequences in  $\Xi$ , and  $\mathcal{B}_\Xi^\mathbb{N}$  is the  $\sigma$ -algebra generated by all cylinder sets of the form

$$\{\bar{\xi} \in \Xi^\mathbb{N} \mid (\bar{\xi}_1, \bar{\xi}_2, \dots, \bar{\xi}_n) \in B\}, \quad B \in \mathcal{B}_\Xi^n,$$

where  $\bar{\xi}_i$  is the  $i$ th entry of the sequence  $\bar{\xi}$ . Correspondingly,  $\mathbb{P}_\theta^\mathbb{N}$  is the product measure that coincides with  $\mathbb{P}_\theta^n$  on  $\mathcal{B}_\Xi^n$ , i.e.,

$$\mathbb{P}_\theta^\mathbb{N}(\{\bar{\xi} \in \Xi^\mathbb{N} \mid (\bar{\xi}_1, \bar{\xi}_2, \dots, \bar{\xi}_n) \in B\}) = \mathbb{P}_\theta^n(B), \quad \forall B \in \mathcal{B}_\Xi^n.$$

Let  $\Omega = \Theta \times \Xi^\mathbb{N}$  be the sample space equipped with the  $\sigma$ -algebra  $\mathcal{F} = \mathcal{B}_\Theta \otimes \mathcal{B}_\Xi^\mathbb{N}$ . We assume that the following holds throughout Chapter 2.

**Assumption 2.1.1.**  $\mathbb{P}_\theta(B)$  is a measurable function of  $\theta$  for all  $B \in \mathcal{B}_\Xi^\mathbb{N}$ .

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<sup>1</sup>For two  $\sigma$ -algebras  $\Sigma_1$  and  $\Sigma_2$ ,  $\Sigma_1 \otimes \Sigma_2$  is defined as  $\sigma(\Sigma_1 \times \Sigma_2)$ .

Under Assumption 3.1.1, we define a measure  $\mu$  on the collection of all rectangle sets in  $\mathcal{F}$  with the following property.

$$\mu(A \times B) := \int_A \int_B \mathbb{P}_\theta^\mathbb{N}(d\xi) \pi(d\theta) = \int_A \mathbb{P}_\theta^\mathbb{N}(B) \pi(d\theta), \quad \forall A \in \mathcal{B}_\Theta, B \in \mathcal{B}_\Xi^\mathbb{N}. \quad (2.1.4)$$

The integrals in (2.1.4) are well-defined by Assumption 3.1.1. Moreover, since the rectangle sets form a semialgebra (see, e.g., [63, Page 3]), there exists a unique extension of  $\mu$  to  $\mathcal{F}$  by Carathéodory's Extension Theorem (see, e.g., [63, Theorem A.1.3]).

**Proposition 2.1.1.** *For any  $C \in \mathcal{F}$ , we have  $\mu(C) = \int_\Theta \mathbb{P}_\theta^\mathbb{N}(C_\theta) \pi(d\theta)$ , where  $C_\theta$  is defined as  $\{\bar{\xi} \in \Xi^\mathbb{N} : (\theta, \bar{\xi}) \in C\}$ .*

*Proof.* Let  $\mathcal{L} := \{C \in \mathcal{F} \mid \mu(C) = \int_\Theta \mathbb{P}_\theta^\mathbb{N}(C_\theta) \pi(d\theta)\}$  and  $\mathcal{P} := \{A \times B \mid A \in \Theta, B \in \Xi^\mathbb{N}\}$ . Then  $\mathcal{L}$  is a  $\lambda$ -system and  $\mathcal{P}$  is a  $\pi$ -system. From (2.1.4) we know  $\mathcal{P} \subseteq \mathcal{L}$ , so  $\mathcal{F} = \sigma(\mathcal{P}) \subseteq \mathcal{L}$  by Dynkin's  $\pi - \lambda$  Theorem (see, e.g., [63, Theorem A.1.4]).  $\square$

**Remark 2.1.1.** *Proposition 2.1.1 characterizes  $\mu$  for all sets in  $\mathcal{F}$ . Loosely speaking,  $\mu$  is the joint distribution of  $\tilde{\theta}$  and an infinite sequence  $\{\xi_i\}$  that is i.i.d. conditioned on  $\tilde{\theta}$ . An important observation is that if  $C \in \mathcal{F}$  has  $\mu(C) = 1$ , then  $\mathbb{P}_\theta(C_\theta) = 1$  for all  $\theta \in \Theta$  up to a set of measure 0 under  $\pi$ . This particular mode of convergence is due to  $1 = \mu(C) = \int_\Theta \mathbb{P}_\theta(C_\theta) \pi(d\theta)$ .*

It remains to define  $\tilde{\theta}$  and  $\xi_i$  as random variables on  $(\Omega, \mathcal{F}, \mu)$ . Take  $\omega \in \Omega$  and write  $\omega$  as  $(\omega_\theta, \omega_\xi)$  such that  $\omega_\theta \in \Theta$  and  $\omega_\xi \in \Xi^\mathbb{N}$ . Define  $\tilde{\theta}(\omega) := \omega_\theta$  and  $\xi_i(\omega) := (\omega_\xi)_i$ , where  $(\cdot)_i$  extracts the  $i$ th entry of a sequence. Under this type of construction, every realization  $\omega$  yields a parameter  $\tilde{\theta}$  and an infinite sequence  $\{\xi_i\}$ . Furthermore, it can be verified that conditioned on  $\tilde{\theta}$ ,  $\{\xi_i\}$  are i.i.d. samples from  $\mathbb{P}_{\tilde{\theta}}$ . The Bayes estimator (under a quadratic loss function) can be expressed by  $\mathbb{E}_\mu[\tilde{\theta} \mid \mathcal{F}_n]$ , where  $\mathcal{F}_n := \sigma(\xi_1, \dots, \xi_n)$  is the filtration generated by data, and the posterior distribution of  $\tilde{\theta}$  is given by  $\mathbb{P}_n(\cdot) := \mu(\{\omega \in \Omega \mid \tilde{\theta}(\omega) \in \cdot\} \mid \mathcal{F}_n)$ .

### 2.1.3 Bayesian Risk Optimization

Under the parametric assumption on  $\mathbb{P}^c$  in Section 2.1.2, we define the following function for notational brevity.

$$H(x, \theta) := \mathbb{E}_{\mathbb{P}_\theta}[h(x, \xi)]. \quad (2.1.5)$$

In practice, the error in estimating  $H$  via Monte-Carlo simulation needs to be taken into consideration. However, to keep our main messages uncluttered from an extra layer of uncertainty, we assume that  $H$  can be evaluated accurately for any pair of  $(x, \theta)$ . Using (2.1.5), the optimization problems (2.1.1) and (2.1.3) can be rewritten as

$$\min_{x \in \mathcal{X}} H(x, \theta^c) \quad \text{and} \quad \min_{x \in \mathcal{X}} \max_{\theta \in \tilde{\Theta}} H(x, \theta), \quad (2.1.6)$$

respectively, where  $\tilde{\Theta}$  is a subset of  $\Theta$ . We assume that  $H$  is finite for every pair  $(x, \theta) \in \mathcal{X} \times \Theta$ . Notice that a well-designed  $\tilde{\Theta}$  in (2.1.6) should reflect the level of uncertainty in the data to infer  $\theta^c$ . For example, it is preferable if the diameter of  $\tilde{\Theta}$  shrinks as more data are observed. Meanwhile, we know from Bayesian asymptotic theory that the posterior converges weakly to a point mass on  $\theta^c$  at an exponential rate [64]. This motivates the idea of using the posterior distribution of  $\tilde{\theta}$  to capture the degree of parameter uncertainty, which leads to the following BRO problem.

$$\min_{x \in \mathcal{X}} \rho_{\mathbb{P}_n} [H(x, \theta)]. \quad (2.1.7)$$

In (2.1.7),  $\rho$  is a risk functional which is defined as a mapping from a random variable to a real number, and  $\mathbb{P}_n$  is the posterior distribution of  $\tilde{\theta}$  given  $n$  data samples. In particular, a risk functional that is subadditive, monotonically increasing, positive homogenous and translation-invariant is called a *coherent risk measure*. We refer the reader to [65, 66, 67] and the references therein for an axiomatic definition of coherent risk measures and its related discussions. Numerous choices of  $\rho$  can be applied to (2.1.7). We follow [28] and

investigate the following four of them.

1. The mean and mean-variance formulations:

$$\min_{x \in \mathcal{X}} \mathbb{E}_{\mathbb{P}_n} [H(x, \theta)] + w \text{Var}_{\mathbb{P}_n} [H(x, \theta)], \quad w \geq 0.$$

2. The value-at-risk (VaR) formulation:

$$\min_{x \in \mathcal{X}} \text{VaR}_{\mathbb{P}_n}^{\alpha} [H(x, \theta)], \quad \alpha \in (0, 1).$$

3. The conditional value-at-risk (CVaR) formulation:

$$\min_{x \in \mathcal{X}} \text{CVaR}_{\mathbb{P}_n}^{\alpha} [H(x, \theta)], \quad \alpha \in (0, 1).$$

In particular, VaR and CVaR are two commonly used risk measures in financial engineering for controlling large loss. For a random variable  $X$ ,  $\text{VaR}^{\alpha}(X)$  is defined as the  $\alpha$ -quantile of  $X$ , i.e.,

$$\text{VaR}^{\alpha}(X) := \inf\{t : \mathbb{P}(X \leq t) \geq \alpha\},$$

and CVaR is defined as the expected loss beyond VaR,

$$\text{CVaR}^{\alpha}(X) := \frac{1}{1 - \alpha} \int_{\alpha}^1 \text{VaR}^r(X) dr.$$

When  $\mathbb{P}(X = \text{VaR}^{\alpha}(X)) = 0$ , CVaR can also be written as a conditional expectation,

$$\text{CVaR}^{\alpha}(X) := \mathbb{E}[X \mid X \geq \text{VaR}^{\alpha}(X)]. \quad (2.1.8)$$

A risk functional is called *law-invariant* if it depends only on the distribution of the random variable. We remark that all four choices of  $\rho$  considered here are law-invariant. Furthermore, mean and CVaR are coherent risk measures; VaR is a risk measure but is not

coherent because it is not subadditive; mean-variance is not a risk measure for its lack of monotonicity.

Some connections between BRO and DRO are drawn as follows. First, coherent risk measures can be represented as optimization problems using duality theory (see, e.g, [67, Section 6.3]), which allows for a DRO interpretation in terms of ambiguity sets. Second, it is possible to reformulate a BRO as a DRO problem. For example, let  $\rho$  be VaR with a risk level  $\alpha$ . Suppose that  $H$  is continuous on  $\mathcal{X} \times \Theta$ ,  $\Theta$  is compact and  $\mathbb{P}_n$  has a positive density on  $\Theta$ , then for  $\alpha = 100\%$ , (2.1.7) can be rewritten as

$$\min_{x \in \mathcal{X}} \text{VaR}_{\mathbb{P}_n}^{100\%} [H(x, \theta)] = \min_{x \in \mathcal{X}} \max_{\theta \in \Theta} H(x, \theta), \quad (2.1.9)$$

where the right hand side (RHS) corresponds to DRO with  $\Theta$  being viewed as an ambiguity set of  $\theta^c$ . It can also be observed that by adjusting the risk level  $\alpha$ , the VaR objective can easily accommodate a wide range of risk preferences from being overly optimistic to being highly risk-averse.

We highlight a few main results before proceeding to the proofs. Let  $\mathcal{N}$  denote a normal distribution, and let  $\phi$  and  $\Phi$  denote  $\mathcal{N}(0, 1)$ 's density and cumulative distribution function, respectively. We use “ $\Rightarrow$ ” to denote weak convergence (see (2.2.1)). The following results are in the pointwise sense, i.e., they hold for every fixed  $x \in \mathcal{X}$ . Specifically, as  $n \rightarrow \infty$ ,

- (i) for the mean and mean-variance objectives,

$$\sqrt{n} \{ \mathbb{E}_{\mathbb{P}_n} [H(x, \theta)] + w \text{Var}_{\mathbb{P}_n} [H(x, \theta)] - H(x, \theta^c) \} \Rightarrow \mathcal{N}(0, \sigma_x^2);$$

- (ii) for the VaR objective,

$$\sqrt{n} \{ \text{VaR}_{\mathbb{P}_n}^\alpha [H(x, \theta)] - H(x, \theta^c) \} \Rightarrow \mathcal{N}(\sigma_x \Phi^{-1}(\alpha), \sigma_x^2);$$



(iii) for the CVaR objective,

$$\sqrt{n} \{ \text{CVaR}_{\mathbb{P}_n}^\alpha [H(x, \theta)] - H(x, \theta^c) \} \Rightarrow \mathcal{N} \left( \frac{\sigma_x}{1 - \alpha} \phi(\Phi^{-1}(\alpha)), \sigma_x^2 \right).$$

In (i)-(iii), the limiting variance in the RHS is defined as

$$\sigma_x^2 := \nabla_\theta H(x, \theta^c)^\top [I(\theta^c)]^{-1} \nabla_\theta H(x, \theta^c),$$

where  $\nabla_\theta H(x, \theta^c)$  is the gradient of  $H(x, \cdot)$  at  $\theta^c$ , the superscript “ $\top$ ” stands for transpose, and  $I(\theta^c)$  is the Fisher information that  $\xi_i$  carries about  $\theta^c$ . An immediate consequence of (i)-(iii) is that confidence intervals (CIs) can be constructed for  $H(x, \theta^c)$ , which is the true objective value. More importantly, as we will show in Section 2.4, these results imply that the objectives of BRO problems are approximately equivalent to a weighted sum of posterior mean objective and the (squared) half-width of the true objective’s CI. In other words, BRO essentially seeks to balance the trade-off between posterior mean performance and the robustness in actual performance.

## 2.2 Consistency of Bayesian Risk Optimization

Since IU diminishes as  $n \rightarrow \infty$ , one naturally expects the objectives of BRO problems to recover the true objective  $H(\cdot, \theta^c)$ , and the optimal solutions of BRO problems to converge to the true optimal solutions. Let  $D_{KL}(P||Q)$  denote the K-L divergence between two distributions  $P$  and  $Q$ , and let “a.s.” be short for “almost surely”. The following assumption is made to guarantee the strong consistency of posterior distribution.

**Assumption 2.2.1** (Sufficient conditions for consistency under  $\mathbb{P}_{\theta^c}^\mathbb{N}$ ).

(i)  $\Theta$  is a compact set.

(ii) For all  $n$ ,  $\mathbb{P}_\theta^n(\cdot)$ <sup>2</sup> has a density  $p_\theta^n(\cdot)$  that is  $\mathcal{B}_\Theta \otimes \mathcal{B}_\Xi$ -measurable.

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<sup>2</sup>Recall from Section 2.1.2 that  $\mathbb{P}_\theta^n$  is defined as the product measure of  $n$  copies of  $\mathbb{P}_\theta$ .

(iii) For any neighborhood  $V \in \mathcal{B}_\Theta$  of  $\theta^c$ , there exists a sequence of uniformly consistent tests of the hypothesis  $\tilde{\theta} = \theta^c$  against the alternative  $\tilde{\theta} \in \Theta \setminus V$ <sup>3</sup>.

(iv) For any  $\epsilon > 0$  and any neighborhood  $V \in \mathcal{B}_\Theta$  of  $\theta^c$ ,  $V$  contains a subset  $W$  such that  $\pi(W) > 0$  and  $D_{KL}(p_{\theta^c} \| p_\theta) < \epsilon$  for all  $\theta \in W$ .

**Lemma 2.2.1** (Theorem 6.1 in [62]). *Suppose Assumption 2.2.1 holds. Then for any neighborhood  $V \in \mathcal{B}_\Theta$  of  $\theta^c$ ,  $\mathbb{P}_n(V) \rightarrow 1$  a.s.  $(\mathbb{P}_{\theta^c}^{\mathbb{N}})$  as  $n \rightarrow \infty$ .*

### 2.2.1 Consistency of Objective Functions

The pointwise weak consistency of BRO problems' objectives has been shown in [28]. We strengthen this result by proving the pointwise strong consistency of BRO problems' objectives, where the proof technique differs from that in [28]. Moreover, our result is essential to establishing the consistency of optimal solutions.

**Definition 2.2.1** (Weak convergence). *A sequence of random variables  $\{X_n\}$  is said to converge weakly (or in distribution) to  $X$ , denoted by  $X_n \Rightarrow X$ , if and only if  $\mathbb{E}[g(X_n)] \rightarrow \mathbb{E}[g(X)]$  as  $n \rightarrow \infty$  for all  $g$  bounded and continuous. Similarly, a sequence of distributions  $\bar{\mathbb{P}}_n \Rightarrow \bar{P}$  if and only if  $\int g(\omega) \bar{\mathbb{P}}_n(d\omega) \rightarrow \int g(\omega) \bar{\mathbb{P}}(d\omega)$  as  $n \rightarrow \infty$  for all  $g$  bounded and continuous.*

**Lemma 2.2.2.** *Suppose Assumption 2.2.1 holds. Then  $\mathbb{P}_n \Rightarrow \delta_{\theta^c}$  a.s.  $(\mathbb{P}_{\theta^c}^{\mathbb{N}})$ , where  $\delta_{\theta^c}$  is a point mass on  $\theta^c$ .*

*Proof.* Let  $\Theta_m \subseteq \Theta$  be an open ball centered at  $\theta^c$  with radius  $1/m$ . Lemma 2.2.1 ensures that for each  $\Theta_m$  there exists an event  $\Omega_m \in \mathcal{B}_{\Xi}^{\mathbb{N}}$  with  $\mathbb{P}_{\theta^c}^{\mathbb{N}}(\Omega_m) = 1$  such that  $\mathbb{P}_n(\Theta_m) \rightarrow 1$  as  $n \rightarrow \infty$  on  $\Omega_m$ . Define  $\tilde{\Omega} := \cap_{m=1}^{\infty} \Omega_m$ , then  $\mathbb{P}_{\theta^c}^{\mathbb{N}}(\tilde{\Omega}) = 1$  and it suffices to show  $\mathbb{P}_n \Rightarrow \delta_{\theta^c}$  on  $\tilde{\Omega}$ . Take a sample path  $\omega \in \tilde{\Omega}$ . Notice that for any bounded and continuous function  $g$

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<sup>3</sup>This condition implies separability of  $\theta^c$  from  $\Theta \setminus V$ . For more details on uniformly consistent tests, we refer the reader to [62].

and a fixed positive integer  $k$ ,  $\mathbb{P}_n(\Theta \setminus \Theta_k) \rightarrow 0$  and thus  $\int_{\Theta \setminus \Theta_k} g(\theta) \mathbb{P}_n(d\theta) \rightarrow 0$  as  $n \rightarrow \infty$ .

It follows that

$$\inf_{\theta \in \Theta_k} g(\theta) \leq \liminf_{n \rightarrow \infty} \int_{\Theta} g(\theta) \mathbb{P}_n(d\theta) \leq \limsup_{n \rightarrow \infty} \int_{\Theta} g(\theta) \mathbb{P}_n(d\theta) \leq \sup_{\theta \in \Theta_k} g(\theta).$$

Letting  $k \rightarrow \infty$ , the continuity of  $g$  and Definition 2.2.1 implies that  $\mathbb{P}_n \Rightarrow \delta_{\theta^c}$ . □

**Theorem 2.2.1.** *Suppose Assumption 2.2.1 holds, and  $H(x, \cdot)$  is continuous on  $\Theta$  for every  $x \in \mathcal{X}$ . Then for every fixed  $x \in \mathcal{X}$ , we have  $\rho_{\mathbb{P}_n}[H(x, \theta)] \rightarrow H(x, \theta^c)$  as  $n \rightarrow \infty$  a.s. ( $\mathbb{P}_{\theta^c}^{\mathbb{N}}$ ) for all four choices of  $\rho$ .*

*Proof.* Suppress  $x$  and write  $H(x, \theta)$  as  $H(\theta)$  for short. We will focus on the same event  $\tilde{\Omega}$  constructed in the proof of Lemma 2.2.2. Take a sample path  $\omega \in \tilde{\Omega}$ . The consistency for each choice of  $\rho$  is shown as follows.

**Mean.** The compactness of  $\Theta$  and the continuity of  $H$  implies that  $H$  is bounded on  $\Theta$ . It follows directly from Definition 2.2.1 that  $\mathbb{E}_{\mathbb{P}_n}[H(\theta)] \rightarrow H(\theta^c)$ .

**Mean-variance.** Since  $\text{Var}_{\mathbb{P}_n}[H(\theta)] = \mathbb{E}_{\mathbb{P}_n}\{[H(\theta)]^2\} - \{\mathbb{E}_{\mathbb{P}_n}[H(\theta)]\}^2$ , where  $H^2$  and  $H$  are bounded and continuous functions, it follows from Definition 2.2.1 that  $\text{Var}_{\mathbb{P}_n}[H(\theta)] \rightarrow [H(\theta^c)]^2 - [H(\theta^c)]^2 = 0$ .

**VaR.** Let  $\mathbb{P}_H^n := \mathbb{P}_n \circ H^{-1}$  be the distribution of  $H(\theta)$  induced by  $\mathbb{P}_n$ . Then  $\mathbb{P}_H^n \Rightarrow \delta_{H(\theta^c)}$  by Continuous Mapping Theorem (see, e.g., [63, Theorem 3.2.4]). Since  $H(\theta^c) - \epsilon$  and  $H(\theta^c) + \epsilon$  are continuity points of  $\delta_{H(\theta^c)}$ , we have for any  $\epsilon > 0$  that

$$\mathbb{P}_H^n(H(\theta) \leq H(\theta^c) - \epsilon) \rightarrow 0 \leq \alpha, \quad \mathbb{P}_H^n(H(\theta) \leq H(\theta^c) + \epsilon) \rightarrow 1 \geq \alpha,$$

which implies that  $H(\theta^c) - \epsilon \leq \text{VaR}_{\mathbb{P}_n}^\alpha[H(\theta)] \leq H(\theta^c) + \epsilon$  for all  $n$  sufficiently large. The convergence follows from that  $\epsilon$  can be chosen arbitrarily small.

**CVaR.** By CVaR's translation invariance and monotonicity,

$$\begin{aligned}
|\text{CVaR}_{\mathbb{P}_n}^\alpha[H(\theta)] - H(\theta^c)| &\leq \text{CVaR}_{\mathbb{P}_n}^\alpha[|H(\theta) - H(\theta^c)|] \\
&= \frac{1}{1-\alpha} \mathbb{E}_{\mathbb{P}_n}[|H(\theta) - H(\theta^c)| \mathbb{1}_{\{|H(\theta) - H(\theta^c)| \geq v_\alpha\}}] \\
&\leq \frac{1}{1-\alpha} \mathbb{E}_{\mathbb{P}_n}[|H(\theta) - H(\theta^c)|],
\end{aligned}$$

where  $\mathbb{1}(\cdot)$  is an indicator function and  $v_\alpha := \text{VaR}_{\mathbb{P}_n}^\alpha[|H(\theta) - H(\theta^c)|]$ . The proof is complete by noting that  $|H(\cdot) - H(\theta^c)|$  is bounded and continuous on  $\Theta$ .  $\square$

### 2.2.2 Consistency of Optimal Solutions

Let  $S_n := \arg \min_{x \in \mathcal{X}} \rho_{\mathbb{P}_n}[H(x, \theta)]$  be the set of optimal solutions of a BRO problem, and let  $S := \arg \min_{x \in \mathcal{X}} H(x, \theta)$  be the set of true optimal solutions. We consider the following deviation between  $S_n$  and  $S$ .

**Definition 2.2.2.** For  $A, B \subseteq \mathcal{X}$ , define  $\mathbb{D}(A, B) := \sup_{x \in A} \text{dist}(x, B)$ , where  $\text{dist}(x, B) := \inf_{y \in B} \|x - y\|$  and  $\|\cdot\|$  denotes an arbitrary norm.

The Hausdorff metric is defined as  $\max\{\mathbb{D}(A, B), \mathbb{D}(B, A)\}$ , but it suffices for us to consider  $\mathbb{D}$ . We will assume that  $\mathcal{X}$  is compact, which is not a strong assumption since the optimal solutions are often contained in a compact set.

**Assumption 2.2.2** (Sufficient conditions for consistency under  $\mu$ ).

- (i)  $\{\Xi, \mathcal{B}_\Xi\}$  and  $\{\Theta, \mathcal{B}_\Theta\}$  are both isomorphic to Borel sets in a complete separable space.
- (ii) If  $\theta_1 \neq \theta_2$ , then there exists a set  $A \in \mathcal{B}_\Xi^\mathbb{N}$  for which  $\mathbb{P}_{\theta_1}(A) \neq \mathbb{P}_{\theta_2}(A)$ .

By Doob's Consistency Theorem [68], Assumption 2.2.2 implies that for any neighborhood  $V \in \mathcal{B}_\Theta$  of  $\theta^c$ ,  $\mathbb{P}_n(V) \rightarrow 1$  a.s. ( $\mu$ ) as  $n \rightarrow \infty$ , which is weaker than Assumption 2.2.1

(see Remark 2.1.1 for a comparison between  $\mu$  and  $\mathbb{P}_{\theta^c}^{\mathbb{N}}$ ) because Assumption 2.2.2 is significantly less stringent than Assumption 2.2.1. However, notice that working with measure  $\mu$  allows an expression of posterior mean as a conditional expectation, where Martingale Convergence Theorem can be applied. The following lemmas will be useful in showing that  $\mathbb{D}(S_n, S) \rightarrow 0$  a.s. ( $\mu$ ) as  $n \rightarrow \infty$ .

**Lemma 2.2.3** (Theorem 5.3 in [67]). *Let  $\mathcal{X}$  be a compact subset of  $\mathbb{R}^d$ . Suppose a sequence of continuous functions  $\{f_n\} : \mathcal{X} \rightarrow \mathbb{R}$  converges uniformly to a continuous function  $f$ . Let  $\bar{S}_n := \arg \min_{x \in \mathcal{X}} f_n(x)$  and  $\bar{S} := \arg \min_{x \in \mathcal{X}} f(x)$ . Then  $\mathbb{D}(\bar{S}_n, \bar{S}) \rightarrow 0$  as  $n \rightarrow \infty$ . Furthermore, we have  $f_n^* \rightarrow f^*$ , where  $f_n^* := \min_{x \in \mathcal{X}} f_n(x)$  and  $f^* := \min_{x \in \mathcal{X}} f(x)$ .*

**Lemma 2.2.4** (Exercise 9.4.10 in [69]). *Let  $\mathcal{X}$  be a compact subset of  $\mathbb{R}^d$ . If  $\{f_n\} : \mathcal{X} \rightarrow \mathbb{R}$  is a sequence of functions converging pointwise to a function  $f$ , and there exists a common Lipschitz constant  $L > 0$  for  $\{f_n\}$  and  $f$ , then  $f_n \rightarrow f$  uniformly.*

**Lemma 2.2.5.** *Let  $X, Y$  be two random variables in  $\mathcal{L}^\infty(\Omega, \mathcal{F}, \mathbb{P})$ , i.e., the space of all essentially bounded random variables. For  $\rho$  a risk functional with monotonicity and translation invariance,  $|\rho(X) - \rho(Y)| \leq \|X - Y\|_\infty$ , where  $\|\cdot\|_\infty$  is the  $L^\infty$  norm. If furthermore  $\rho$  is a coherent risk measure, then  $|\rho(X) - \rho(Y)| \leq \rho(|X - Y|)$ .*

*Proof.* See [70, Lemma 4.3] for proof of the first part. For the second part, by subadditivity  $\rho(Y) + \rho(X - Y) \geq \rho(X)$ , and by monotonicity  $\rho(X) - \rho(Y) \leq \rho(X - Y) \leq \rho(|X - Y|)$ . The result follows by symmetry.  $\square$

**Theorem 2.2.2.** *Suppose that Assumption 2.2.2 holds,  $\Theta$  and  $\mathcal{X}$  are compact, and  $H(x, \cdot)$  is continuous on  $\Theta$  for every  $x \in \mathcal{X}$ . If*

- (i) *for mean and CVaR, there exists a measurable function  $\kappa : \Theta \rightarrow \mathbb{R}^+$  with  $|H(x, \theta) - H(y, \theta)| \leq \kappa(\theta)\|x - y\|$ ,  $\forall x, y \in \mathcal{X}$  and  $\int_\Theta \kappa(\theta)\pi(d\theta) < \infty$ ;*
- (ii) *for mean-variance,  $H$  is jointly continuous on  $\mathcal{X} \times \Theta$ ;*
- (iii) *for VaR, (i) holds with  $\|\kappa\|_\infty < \infty$ ,*

then for all four choices of  $\rho$ ,

$$\mathbb{D}(S_n, S) \rightarrow 0 \quad \text{a.s. } (\mu), \quad \text{and}$$

$$\min_{x \in \mathcal{X}} \rho_{\mathbb{P}_n}[H(x, \theta)] \rightarrow \min_{x \in \mathcal{X}} H(x, \theta^c) \quad \text{a.s. } (\mu) \quad \text{as } n \rightarrow \infty.$$

*Proof.* The following argument is in the sense of a.s.  $(\mu)$ . Similar to the proof of Theorem 2.2.1, it can be shown that  $\rho_{\mathbb{P}_n}[H(\cdot, \theta)] \rightarrow H(\cdot, \theta^c)$  pointwise on  $\mathcal{X}$  as  $n \rightarrow \infty$ . If we further show that  $\rho_{\mathbb{P}_n}[H(\cdot, \theta)]$  has a common Lipschitz constant  $L$  for all  $n$ , then Lemma 2.2.4 implies that  $\rho_{\mathbb{P}_n}[H(\cdot, \theta)] \rightarrow H(\cdot, \theta^c)$  uniformly on  $\mathcal{X}$ , and the conclusion is an immediate consequence of Lemma 2.2.3.

**Mean.** Recall from Section 2.1.2 that the posterior mean can be expressed as a conditional expectation. Thus, we have for all  $x, y \in \mathcal{X}$ ,

$$|\mathbb{E}_{\mathbb{P}_n}[H(x, \theta)] - \mathbb{E}_{\mathbb{P}_n}[H(y, \theta)]| \leq \mathbb{E}_{\mu}[\kappa(\theta) \mid \mathcal{F}_n] \|x - y\|.$$

By assumption  $\mathbb{E}_{\mu}[|\kappa(\theta)|] = \int \kappa(\theta) \pi(d\theta) < \infty$ , so  $\mathbb{E}_{\mu}[\kappa(\theta) \mid \mathcal{F}_n]$  is a Doob martingale and by Martingale Convergence Theorem (see, e.g., [63, Theorem 5.5.7]),

$$\mathbb{E}_{\mu}[\kappa(\theta) \mid \mathcal{F}_n] \rightarrow \mathbb{E}_{\mu}[\kappa(\theta) \mid \mathcal{F}_{\infty}] \quad \text{as } n \rightarrow \infty,$$

where  $\mathcal{F}_{\infty} := \sigma(\cup_n \mathcal{F}_n)$ . Since  $\mathbb{E}_{\mu}\{\mathbb{E}_{\mu}[\kappa(\theta) \mid \mathcal{F}_{\infty}]\} = \mathbb{E}_{\mu}[\kappa(\theta)] < \infty$ ,  $\mathbb{E}_{\mu}[\kappa(\theta) \mid \mathcal{F}_{\infty}]$  is a.s. finite, and there exists an  $L := \sup_n \mathbb{E}_{\mu}[\kappa(\theta) \mid \mathcal{F}_n] < \infty$ .

**Mean-variance.** It suffices to find an  $L$  for  $\text{Var}_{\mathbb{P}_n}[H(\cdot, \theta)]$ . By definition,

$$\text{Var}_{\mathbb{P}_n}[H(\cdot, \theta)] = \mathbb{E}_{\mathbb{P}_n} \{ [H(\cdot, \theta)]^2 \} - \{ \mathbb{E}_{\mathbb{P}_n}[H(\cdot, \theta)] \}^2. \quad (2.2.1)$$

Since  $H$  is jointly continuous on  $\mathcal{X} \times \Theta$ ,  $|H| \leq M$  for some  $M \geq 0$ . For the first term in

the RHS of (2.2.1),

$$\begin{aligned}\mathbb{E}_{\mathbb{P}_n} \{ [H(x, \theta)]^2 - [H(y, \theta)]^2 \} &\leq \mathbb{E}_{\mathbb{P}_n} \{ |H(x, \theta) + H(y, \theta)| \cdot |H(x, \theta) - H(y, \theta)| \} \\ &\leq 2M \mathbb{E}_{\mathbb{P}_n} \{ |H(x, \theta) - H(y, \theta)| \}.\end{aligned}$$

Similarly, for the second term,

$$\begin{aligned}&| \{ \mathbb{E}_{\mathbb{P}_n} [H(x, \theta)] \}^2 - \{ \mathbb{E}_{\mathbb{P}_n} [H(y, \theta)] \}^2 | \\ &\leq | \mathbb{E}_{\mathbb{P}_n} [H(x, \theta)] + \mathbb{E}_{\mathbb{P}_n} [H(y, \theta)] | \cdot | \mathbb{E}_{\mathbb{P}_n} [H(x, \theta)] - \mathbb{E}_{\mathbb{P}_n} [H(y, \theta)] | \\ &\leq 2M | \mathbb{E}_{\mathbb{P}_n} [H(x, \theta)] - \mathbb{E}_{\mathbb{P}_n} [H(y, \theta)] |,\end{aligned}$$

and the rest follows from the case of mean.

**VaR.** Since  $\|\kappa\|_\infty < \infty$ , there exists  $L > 0$  such that  $|H(x, \theta) - H(y, \theta)| \leq L\|x - y\|$  for all  $x, y \in \mathcal{X}$  and  $\theta \in \Theta$ . By the first part of Lemma 2.2.5,

$$| \text{VaR}_{\mathbb{P}_n}^\alpha [H(x, \theta)] - \text{VaR}_{\mathbb{P}_n}^\alpha [H(y, \theta)] | \leq \|H(x, \theta) - H(y, \theta)\|_\infty \leq L\|x - y\|.$$

**CVaR.** Using the second part of Lemma 2.2.5, we have for any  $x, y$  in  $\mathcal{X}$ ,

$$| \text{CVaR}_{\mathbb{P}_n}^\alpha [H(x, \theta)] - \text{CVaR}_{\mathbb{P}_n}^\alpha [H(y, \theta)] | \leq \frac{1}{1 - \alpha} \mathbb{E}_\mu[\kappa(\theta) \mid \mathcal{F}_n] \|x - y\|,$$

and the rest follows from the proof of the mean formulation.  $\square$

As a special case, convex functions have the following nice property regarding uniform convergence: if a sequence of convex functions converges pointwise on an open set  $O \subset \mathbb{R}^n$ , then it also converges uniformly on any compact subset of  $O$  (see, e.g., [71, Theorem 3.1.4]). This leads to the following corollary of Theorem 2.2.1 for convex risk measures (e.g., mean and CVaR).

**Corollary 2.2.1.** *Suppose Assumption 2.2.1 holds, and  $H(x, \cdot)$  is continuous on  $\Theta$  for every  $x \in \mathcal{X}$ . Also let  $H(\cdot, \theta)$  be convex in  $x$  for all  $\theta \in \Theta$ , then for the mean and the CVaR formulations, we have  $\mathbb{D}(S_n, S) \rightarrow 0$  a.s. ( $\mathbb{P}_{\theta^c}^{\mathbb{N}}$ ).*

### 2.3 Asymptotic Normality of Objectives

We present two types of asymptotic normality results in this section. First, we show for a fixed  $x$  that  $\sqrt{n}\{\rho_{\mathbb{P}_n}[H(x, \theta)] - H(x, \theta^c)\}$  converges weakly to a normal distribution. Then, we extend this result by establishing weak convergence of  $\sqrt{n}\{\rho_{\mathbb{P}_n}[H(\cdot, \theta)] - H(\cdot, \theta^c)\}$  in the space of continuous functions. To begin with, define  $Z_n(\theta) := \sqrt{n}(\theta - \theta^c)$  and let  $\mathbb{P}_{Z_n} := \mathbb{P}_n \circ Z_n^{-1}$  be the distribution of  $Z_n$  induced by  $\mathbb{P}_n$ .

**Definition 2.3.1.** *For two probability measures  $\mu$  and  $\nu$  on a measurable space  $(\Omega, \mathcal{F})$ , their total variation distance is defined as  $\|\mu - \nu\|_{TV} := \sup_{A \in \mathcal{F}} |\mu(A) - \nu(A)|$ .*

**Lemma 2.3.1** (Bernstein-von Mises Theorem). *Under mild conditions,*

$$\|\mathbb{P}_{Z_n} - \mathcal{N}(\Delta_n, [I(\theta^c)]^{-1})\|_{TV} \rightarrow 0 \text{ in probability } (\mathbb{P}_{\theta^c}^{\mathbb{N}}) \text{ as } n \rightarrow \infty, \quad (2.3.1)$$

where  $\mathcal{N}$  denotes a normal distribution,  $I(\theta^c)$  is the Fisher information  $\xi_i$  carries about  $\theta^c$ , and  $\Delta_n \Rightarrow \mathcal{N}(0, [I(\theta^c)]^{-1})$  as  $n \rightarrow \infty$ .

We refer the reader to [72, Theorem 10.1] for detailed conditions of Lemma 2.3.1, which are mild and are assumed to hold in all subsequent proofs. We remark that Lemma 2.3.1 is also commonly referred to as the Bayesian Central Limit Theorem. Recall that we consider a law-invariant  $\rho$ , so there is no ambiguity in writing  $\rho(\mathbb{P})$  for some distribution  $\mathbb{P}$ . The forthcoming proofs of asymptotic normality are motivated by the following heuristic argument.

**Step 1.** If  $\rho$  is translation-invariant and positive homogeneous, then

$$\sqrt{n}\{\rho_{\mathbb{P}_n}[H(x, \theta)] - H(x, \theta^c)\} = \rho_{\mathbb{P}_n}\{\sqrt{n}[H(x, \theta) - H(x, \theta^c)]\} \approx \rho_{\mathbb{P}_n}[X_n(\theta)], \quad (2.3.2)$$



where  $X_n(\theta) := \nabla_\theta H(x, \theta^c)^\top Z_n(\theta)$  is the first-order Taylor approximation.

**Step 2.** Based on Lemma 2.3.1, show that

$$\|\mathbb{P}_n \circ X_n^{-1} - \mathcal{N}(\nabla_\theta H(x, \theta^c)^\top \Delta_n, \sigma_x^2)\|_{\text{TV}} \rightarrow 0 \quad \text{in probability,} \quad (2.3.3)$$

where  $\sigma_x^2 := \nabla_\theta H(x, \theta^c)^\top [I(\theta^c)]^{-1} \nabla_\theta H(x, \theta^c)$ .

**Step 3.** Since  $\rho_{\mathbb{P}_n}(X_n(\theta)) = \rho(\mathbb{P}_n \circ X_n^{-1})$ , it suffices to show that

$$\rho(\mathbb{P}_n \circ X_n^{-1}) - \rho[\mathcal{N}(\nabla_\theta H(x, \theta^c)^\top \Delta_n, \sigma_x^2)] \rightarrow 0 \quad \text{in probability.} \quad (2.3.4)$$

If the above argument holds, then the asymptotic distribution of BRO problems' objectives can be easily characterized since  $\rho[\mathcal{N}(\nabla_\theta H(x, \theta^c)^\top \Delta_n, \sigma_x^2)]$  allows closed forms for all four choices of  $\rho$ . However, each step listed above involves a gap to be closed. In particular, note that  $\mathcal{N}(\nabla_\theta H(x, \theta^c)^\top \Delta_n, \sigma_x^2)$  is not a fixed measure. Thus, from a general perspective, step 3 essentially investigates the following: for two sequences of probability measures  $\{\mu_n\}$  and  $\{\nu_n\}$ , does  $\|\mu_n - \nu_n\|_{\text{TV}} \rightarrow 0$  imply that  $\rho(\mu_n) - \rho(\nu_n) \rightarrow 0$ ? In other words, when  $\rho$  is viewed as a functional of distributions, is it uniformly continuous relative to the total variation metric? Unfortunately, this is not true for our four choices of  $\rho$ . Nevertheless, it is possible for us to exploit the structure of  $\mathcal{N}(\Delta_n, [I(\theta^c)]^{-1})$  to circumvent this issue.

### 2.3.1 Asymptotic Normality at a Fixed $x$

Once  $x$  is fixed, we write  $H(x, \theta)$  as  $H(\theta)$  for notational brevity. Consider  $\|\cdot\|$  being the Euclidean norm henceforth for convenience. In establishing asymptotic normality, each choice of  $\rho$  has distinct properties and deserves separate treatment. To bridge the gaps in the preceding sketch of proof, we need the following regularity condition.

**Assumption 2.3.1.** *There exists a constant  $\gamma > 0$  such that for all  $\epsilon > 0$ , there exists an*

$M_\epsilon > 0$  satisfying

$$\mathbb{P}_{\theta^c}^{\mathbb{N}} \left\{ \mathbb{E}_{\mathbb{P}_n} [\|\sqrt{n}(\theta - \theta^c)\|^{1+\gamma}] > M_\epsilon \right\} < \epsilon, \quad \forall n.$$

Assumption 2.3.1 can be viewed as an “in probability” version of uniform integrability, because on event  $\{\mathbb{E}_{\mathbb{P}_n} [\|\sqrt{n}(\theta - \theta^c)\|^{1+\gamma}] \leq M_\epsilon\}$ , we have

$$\mathbb{E}_{\mathbb{P}_n} [\|\sqrt{n}(\theta - \theta^c)\| \mathbb{1}_{\{\|\sqrt{n}(\theta - \theta^c)\| > K\}}] \leq \frac{\mathbb{E}_{\mathbb{P}_n} [\|\sqrt{n}(\theta - \theta^c)\|^{1+\gamma}]}{K^\gamma} \leq \frac{M_\epsilon}{K^\gamma} \quad (2.3.5)$$

for any  $K > 0$ . Thus, for sufficiently large  $K$ , the truncated tail expectation of  $\|\sqrt{n}(\theta - \theta^c)\|$  can be arbitrarily small with a large probability ( $\mathbb{P}_{\theta^c}^{\mathbb{N}}$ ) for all  $n$ . Another implication is that

$$\mathbb{P}_n(\|\sqrt{n}(\theta - \theta^c)\| > K) \leq \frac{M_\epsilon}{K^{1+\gamma}}$$

by Markov’s inequality. As we will see in the proof of Theorem 2.3.1, Assumption 2.3.1 plays a vital role in bounding the remainder term in Taylor expansion. The following lemma is a special case of [72, Theorem 10.8], where the conditions are implicitly assumed to hold in all subsequent proofs.

**Lemma 2.3.2.** *Under mild assumptions,*

$$\sqrt{n} (\mathbb{E}_{\mathbb{P}_n}[\theta] - \theta^c) \Rightarrow \mathcal{N}(0, [I(\theta^c)]^{-1}), \quad \text{as } n \rightarrow \infty.$$

We now verify Assumption 2.3.1 for some commonly used conjugate priors. Notice that if  $\Theta \subseteq \mathbb{R}$ , then for  $\gamma = 1$ ,

$$\mathbb{E}_{\mathbb{P}_n} \{[\sqrt{n}(\theta - \theta^c)]^2\} = \{\sqrt{n}(\mathbb{E}_{\mathbb{P}_n}[\theta] - \theta^c)\}^2 + n \text{Var}_{\mathbb{P}_n}[\theta],$$

where the first term in the RHS converges in distribution by Lemma 2.3.2, so we only need to check if the second term is bounded in probability ( $\mathbb{P}_{\theta^c}^{\mathbb{N}}$ ).

**Example 2.3.1.** Let  $\xi_i \sim \text{Expo}(\theta^c)$  and  $\pi \sim \text{Gamma}(\alpha_0, \beta_0)$ . Then,  $\mathbb{P}_n$  is given by  $\text{Gamma}(\alpha_n, \beta_n)$ , where  $\alpha_n = \alpha_0 + n$  and  $\beta_n = \beta_0 + \sum_{i=1}^n \xi_i$ . Furthermore,

$$n\text{Var}_{\mathbb{P}_n}[\theta] = \frac{n\alpha_n}{\beta_n^2} = \left( \frac{n}{\beta_0 + \sum_{i=1}^n \xi_i} \right)^2 + \frac{\alpha_0 n}{(\beta_0 + \sum_{i=1}^n \xi_i)^2} \rightarrow (\theta^c)^2 \quad a.s. (\mathbb{P}_{\theta^c}^{\mathbb{N}}),$$

where the convergence follows from the strong law of large numbers (SLLN).

**Example 2.3.2.** Let  $\xi_i \sim \mathcal{N}(\theta^c, \sigma^2)$ , where  $\sigma^2$  is known and  $\pi \sim \mathcal{N}(\mu_0, \sigma_0^2)$ . We then have

$$n\text{Var}_{\mathbb{P}_n}[\theta] = n\sigma_n^2 = \frac{n}{1/\sigma_0^2 + n/\sigma^2} \rightarrow \sigma^2 \quad a.s. (\mathbb{P}_{\theta^c}^{\mathbb{N}}).$$

**Example 2.3.3.** Let  $\xi_i \sim \text{Weibull}(\theta^c, \beta)$ , where  $\theta^c$  is an unknown scale parameter and  $\beta$  is a known shape parameter. Let the posterior of  $\tilde{\theta}^\beta$  be  $\text{InvGamma}(\alpha_n, \beta_n)$ , where  $\alpha_n = \alpha_0 + n$  and  $\beta_n = \beta_0 + \sum_{i=1}^n \xi_i^\beta$ . Then by the SLLN,

$$n\text{Var}_{\mathbb{P}_n}[\theta^\beta] = \frac{n\beta_n^2}{(\alpha_n - 1)^2(\alpha_n - 2)} = \frac{n^3(\beta_0/n + \sum_{i=1}^n \xi_i^\beta/n)^2}{(\alpha_0 + n - 1)^2(\alpha_0 + n - 2)} \rightarrow (\theta^c)^{2\beta} a.s. (\mathbb{P}_{\theta^c}^{\mathbb{N}}).$$

**Example 2.3.4.** Let  $\xi_i$  be a discrete random variable supported on  $\{y_1, \dots, y_l\}$ . Suppose  $\mathbb{P}(\xi_i = y_i) = \theta_i^c$ , then  $\theta^c := (\theta_1^c, \dots, \theta_l^c)$  can be viewed as a parameter in  $\mathbb{R}^l$ . Choose  $\pi \sim \text{Dirichlet}(\alpha_0)$ , where  $\alpha_0 = (1, \dots, 1)$ . It follows that  $\mathbb{P}_n \sim \text{Dirichlet}(\alpha_n)$ , where  $\alpha_n = \alpha_0 + (N_1, \dots, N_l)$  and  $N_i := \sum_{j=1}^n \mathbb{1}_{\{\xi_j = y_i\}}$ . Let  $\theta_i$ ,  $\theta_i^c$  and  $\alpha_i^n$  denote the  $i$ th component of  $\theta$ ,  $\theta^c$  and  $\alpha_n$ , respectively. Since

$$\mathbb{E}_{\mathbb{P}_n} [\|\sqrt{n}(\theta - \theta^c)\|^2] = n \sum_{i=1}^l \mathbb{E}_{\mathbb{P}_n} [(\theta_i - \theta_i^c)^2],$$

it suffices to check the convergence of  $n\mathbb{E}_{\mathbb{P}_n} [(\theta_i - \theta_i^c)^2]$  for each  $i$ . Likewise,

$$n\mathbb{E}_{\mathbb{P}_n} [(\theta_i - \theta_i^c)^2] = n(\mathbb{E}_{\mathbb{P}_n} [\theta_i] - \theta_i^c)^2 + n\text{Var}_{\mathbb{P}_n}(\theta_i),$$

where, by noting  $\sum_{j=1}^l \alpha_j^n = l + n$ , we have

$$\sqrt{n}(\mathbb{E}_{\mathbb{P}_n}[\theta_i] - \theta_i^c) = \sqrt{n} \left( \frac{\alpha_i^n}{l + n} - \theta_i^c \right) = \sqrt{n} \left( \frac{1 + N_i}{l + n} - \theta_i^c \right),$$

which converges weakly by the Central Limit Theorem, and the SLLN implies that

$$n \text{Var}_{\mathbb{P}_n}(\theta_i) = n \frac{\alpha_i^n(l + n - \alpha_i^n)}{(l + n)^2(l + n + 1)} \rightarrow \theta_i^c(1 - \theta_i^c) \quad a.s. \quad (\mathbb{P}_{\theta^c}^{\mathbb{N}}).$$

The proofs of asymptotic normality will be presented in the order of mean, mean-variance, VaR and CVaR. Recall from previous notation that

$$\sigma_x^2 := \nabla_{\theta} H(x, \theta^c)^{\top} [I(\theta^c)]^{-1} \nabla_{\theta} H(x, \theta^c).$$

**Theorem 2.3.1.** *Let Assumptions 2.2.1 and 2.3.1 hold. If  $H$  is continuous on  $\Theta$  and differentiable at  $\theta^c$ , then*

$$\sqrt{n} \{ \mathbb{E}_{\mathbb{P}_n}[H(\theta)] - H(\theta^c) \} \Rightarrow \mathcal{N}(0, \sigma_x^2) \quad \text{as } n \rightarrow \infty.$$

If furthermore Assumption 2.3.1 holds with  $\gamma = 1$ , then as  $n \rightarrow \infty$ ,

$$\sqrt{n} \{ \mathbb{E}_{\mathbb{P}_n}[H(\theta)] + w \text{Var}_{\mathbb{P}_n}[H(\theta)] - H(\theta^c) \} \Rightarrow \mathcal{N}(0, \sigma_x^2).$$

*Proof.* The first-order Taylor expansion of  $H$  around  $\theta^c$  yields

$$\mathbb{E}_{\mathbb{P}_n}[\sqrt{n}(H(\theta) - H(\theta^c))] = \nabla H(\theta^c)^{\top} \mathbb{E}_{\mathbb{P}_n}[\sqrt{n}(\theta - \theta^c)] + \mathbb{E}_{\mathbb{P}_n}[e(\theta) \|\sqrt{n}(\theta - \theta^c)\|], \quad (2.3.6)$$

where  $e(\theta) \rightarrow 0$  if  $\theta \rightarrow \theta^c$ . The first term in the RHS of (2.3.6) converges weakly to

$\mathcal{N}(0, \sigma_x^2)$  by Lemma 2.3.2. Applying Hölder's inequality to the remainder,

$$|\mathbb{E}_{\mathbb{P}_n}[e(\theta)\|\sqrt{n}(\theta - \theta^c)\|]| \leq \left(\mathbb{E}_{\mathbb{P}_n}\left[|e(\theta)|^{\frac{1+\gamma}{\gamma}}\right]\right)^{\frac{\gamma}{1+\gamma}} \left(\mathbb{E}_{\mathbb{P}_n}\left[\|\sqrt{n}(\theta - \theta^c)\|^{1+\gamma}\right]\right)^{\frac{1}{1+\gamma}}.$$

Setting  $e(\theta^c) = 0$  does not affect (2.3.6), so we assume that  $e(\cdot)$  is bounded and continuous on  $\Theta$  by the continuity of  $H$  and the compactness of  $\Theta$ . From Lemma 2.2.2 we know that  $\mathbb{P}_n \Rightarrow \delta_{\theta^c}$  a.s. ( $\mathbb{P}_{\theta^c}^{\mathbb{N}}$ ), thus by Definition 2.2.1,

$$\mathbb{E}_{\mathbb{P}_n}\left[|e(\theta)|^{(1+\gamma)/\gamma}\right] \rightarrow |e(\theta^c)|^{(1+\gamma)/\gamma} = 0 \quad \text{a.s. } (\mathbb{P}_{\theta^c}^{\mathbb{N}}) \quad \text{as } n \rightarrow \infty,$$

which together with Assumption 2.3.1 imply that the remainder converges weakly to 0.

This proves the the case of mean. For mean-variance, we only need to show that  $\sqrt{n}\text{Var}_{\mathbb{P}_n}\{H(\theta)\} \Rightarrow 0$ . Note that

$$\begin{aligned} \sqrt{n}\text{Var}_{\mathbb{P}_n}[H(\theta)] &= \sqrt{n}\text{Var}_{\mathbb{P}_n}[H(\theta) - H(\theta^c)] \leq \sqrt{n}\mathbb{E}_{\mathbb{P}_n}\{[H(\theta) - H(\theta^c)]^2\} \\ &= \sqrt{n}\mathbb{E}_{\mathbb{P}_n}\left[(\nabla H(\theta^c)^\top(\theta - \theta^c) + e(\theta)\|\theta - \theta^c\|)^2\right] \\ &\leq \underbrace{2\sqrt{n}\mathbb{E}_{\mathbb{P}_n}\left[|\nabla H(\theta^c)^\top(\theta - \theta^c)|^2\right]}_{(*)} + \underbrace{2\sqrt{n}\mathbb{E}_{\mathbb{P}_n}\{[e(\theta)]^2\|\theta - \theta^c\|^2\}}_{(**)}, \end{aligned}$$

where the last inequality follows from  $(a + b)^2 \leq 2a^2 + 2b^2$ . Furthermore,

$$(*) \leq \frac{2}{\sqrt{n}}\|\nabla H(\theta^c)\|^2\mathbb{E}_{\mathbb{P}_n}\{\|\sqrt{n}(\theta - \theta^c)\|^2\} \Rightarrow 0 \quad \text{as } n \rightarrow \infty$$

since  $\mathbb{E}_{\mathbb{P}_n}\{\|\sqrt{n}(\theta - \theta^c)\|^2\}$  is bounded in probability ( $\mathbb{P}_{\theta^c}^{\mathbb{N}}$ ) by assumption. Similarly, we have  $(**) \Rightarrow 0$  by the boundedness of  $e(\cdot)$  on  $\Theta$ .  $\square$

**Remark 2.3.1.** *The proof of Theorem 2.3.1 is basically a combination of Lemma 2.3.2 and the Delta method. From definition we know that convergence in total variation implies weak convergence, which together with uniform integrability implies convergence of expectation (see, e.g., [73, Theorem 3.5]). This is the main motivation behind Assumption 2.3.1.*

**Remark 2.3.2.** *A potential alternative way to reach the same conclusion might be based on the nontrivial asymptotic equivalence between Bayes and maximum likelihood estimation (see, e.g., [74, Page 450]), but it could require numerous intricate technical assumptions that can be found in [75].*

For notational ease, let  $\mathbb{P}_X$  denote the distribution of a random variable  $X$ . Also let  $\phi$  and  $\Phi$  be the density and cumulative distribution function of  $\mathcal{N}(0, 1)$ , respectively. The forthcoming proof for VaR is based on a series of lemmas presented in the same order as the steps in the heuristic argument: Lemma 2.3.3 copes with the remainder term in Taylor expansion; Lemma 2.3.4 shows that the total variation distance between two distributions will not increase under reasonable mappings; Lemma 2.3.5 closes the final gap between convergence in total variation and convergence of VaR.

**Lemma 2.3.3.** *Let  $X$  and  $Y$  be two random variables, where  $X$  and  $X + Y$  both have positive densities. Given  $\alpha \in (0, 1)$  and  $\epsilon \in (0, \min\{\alpha, 1 - \alpha\})$ , suppose that  $\mathbb{P}(|Y| > \delta) < \epsilon$  for some  $\delta > 0$ . Then,*

$$\text{VaR}^{\alpha-\epsilon}(X) - \delta \leq \text{VaR}^\alpha(X + Y) \leq \text{VaR}^{\alpha+\epsilon}(X) + \delta.$$

*Proof.* Since  $X$  and  $X + Y$  have positive densities, their cumulative distribution functions are continuous and strictly increasing. Thus,

$$\mathbb{P}(X \leq \text{VaR}^\alpha(X)) = \alpha, \quad \mathbb{P}(X + Y \leq \text{VaR}^\alpha(X + Y)) = \alpha, \quad \forall \alpha \in (0, 1).$$

fully characterizes  $\text{VaR}^\alpha(X)$  and  $\text{VaR}^\alpha(X + Y)$ . The conclusion then follows from the next two observations.

(i)  $\mathbb{P}(X + Y \leq \text{VaR}^{\alpha-\epsilon}(X) - \delta) \leq \alpha :$

$$\begin{aligned} \text{LHS} &\leq \mathbb{P}(X + Y \leq \text{VaR}^{\alpha-\epsilon}(X) - \delta, |Y| \leq \delta) + \mathbb{P}(|Y| > \delta) \\ &\leq \mathbb{P}(X + Y \leq \text{VaR}^{\alpha-\epsilon}(X) - \delta, Y \geq -\delta) + \epsilon \\ &\leq \mathbb{P}(X \leq \text{VaR}^{\alpha-\epsilon}(X)) + \epsilon = \alpha - \epsilon + \epsilon = \alpha. \end{aligned}$$

(ii)  $\mathbb{P}(X + Y \leq \text{VaR}^{\alpha+\epsilon}(X) + \delta) \geq \alpha :$

$$\begin{aligned} \text{LHS} &\geq \mathbb{P}(X \leq \text{VaR}^{\alpha+\epsilon}(X), Y \leq \delta) \\ &\geq 1 - \mathbb{P}(X > \text{VaR}^{\alpha+\epsilon}(X)) - \mathbb{P}(Y > \delta) \\ &\geq \mathbb{P}(X \leq \text{VaR}^{\alpha+\epsilon}(X)) - \epsilon = \alpha + \epsilon - \epsilon = \alpha. \end{aligned}$$

□

**Lemma 2.3.4.** *Let  $X$  and  $Y$  be random variables taking values in a measurable space  $(\Omega, \mathcal{F})$ . Then, for any measurable function  $h : (\Omega, \mathcal{F}) \rightarrow (\tilde{\Omega}, \tilde{\mathcal{F}})$ , we have*

$$\|\mathbb{P}_{h(X)} - \mathbb{P}_{h(Y)}\|_{\text{TV}} \leq \|\mathbb{P}_X - \mathbb{P}_Y\|_{\text{TV}}.$$

*Proof.* For any  $B \in \tilde{\mathcal{F}}$ , we have  $h^{-1}(B) \in \mathcal{F}$  and

$$|\mathbb{P}_{h(X)}(B) - \mathbb{P}_{h(Y)}(B)| = |\mathbb{P}_X(h^{-1}(B)) - \mathbb{P}_Y(h^{-1}(B))| \leq \sup_{A \in \mathcal{F}} |\mathbb{P}_X(A) - \mathbb{P}_Y(A)|,$$

where the last term is  $\|\mathbb{P}_X - \mathbb{P}_Y\|_{\text{TV}}$ . The result follows from taking supremum over  $B \in \tilde{\mathcal{F}}$  on both sides. □

**Lemma 2.3.5.** *If  $X$  is a random variable with positive density,  $Y \sim \mathcal{N}(c, \sigma^2)$ , and  $\|\mathbb{P}_X -$*

$\mathbb{P}_Y\|_{TV} \leq \epsilon$ , where  $\epsilon \in (0, \min\{\alpha, 1 - \alpha\})$  and  $\alpha \in (0, 1)$ , then

$$|\text{VaR}^\alpha(X) - \text{VaR}^\alpha(Y)| \leq \sigma \max\{\Phi^{-1}(\alpha) - \Phi^{-1}(\alpha - \epsilon), \Phi^{-1}(\alpha + \epsilon) - \Phi^{-1}(\alpha)\}.$$

*Proof.* Note that  $\text{VaR}^\alpha(Y) = c + \sigma\Phi^{-1}(\alpha)$ . Since  $\|\mathbb{P}_X - \mathbb{P}_Y\|_{TV} \leq \epsilon$ , we have

$$\mathbb{P}(X \leq \text{VaR}_{\alpha+\epsilon}(Y)) \geq \mathbb{P}(Y \leq \text{VaR}_{\alpha+\epsilon}(Y)) - \epsilon = \alpha + \epsilon - \epsilon = \alpha,$$

$$\mathbb{P}(X \leq \text{VaR}_{\alpha-\epsilon}(Y)) \leq \mathbb{P}(Y \leq \text{VaR}_{\alpha-\epsilon}(Y)) + \epsilon = \alpha - \epsilon + \epsilon = \alpha.$$

Hence  $\text{VaR}^{\alpha-\epsilon}(Y) \leq \text{VaR}^\alpha(X) \leq \text{VaR}^{\alpha+\epsilon}(Y)$ , and the result follows from the closed forms of  $\text{VaR}^{\alpha\pm\epsilon}(Y)$ .  $\square$

**Theorem 2.3.2.** Suppose that Assumptions 2.2.1 and 2.3.1 hold, and  $H$  is differentiable at  $\theta^c$ . Also assume for  $\theta \sim \mathbb{P}_n$  that  $\sqrt{n}(\theta - \theta^c)$  and  $\sqrt{n}[H(\theta) - H(\theta^c)]$  have positive densities for all  $n$  a.s. ( $\mathbb{P}_{\theta^c}^\mathbb{N}$ ). Then for any  $\alpha \in (0, 1)$ ,

$$\sqrt{n} \{ \text{VaR}_{\mathbb{P}_n}^\alpha[H(\theta)] - H(\theta^c) \} \Rightarrow \mathcal{N}(\sigma\Phi^{-1}(\alpha), \sigma_x^2).$$

*Proof.* Since  $x$  is fixed, we write  $\sigma_x^2$  as  $\sigma^2$  for short. Let  $Y_n$  denote a random variable with distribution  $\mathcal{N}(\nabla H(\theta^c)^\top \Delta_n, \sigma^2)$ . Our goal is to show that for any  $\delta, \epsilon > 0$ , there exists  $N > 0$  such that

$$\mathbb{P}_{\theta^c}^\mathbb{N} \{ |\sqrt{n} \{ \text{VaR}_{\mathbb{P}_n}^\alpha[H(\theta)] - H(\theta^c) \} - \text{VaR}^\alpha(Y_n)| > \delta \} < \epsilon, \quad \forall n > N. \quad (2.3.7)$$

By the positive homogeneity and translation invariance of  $\text{VaR}$ ,

$$\sqrt{n} \{ \text{VaR}_{\mathbb{P}_n}^\alpha[H(\theta)] - H(\theta^c) \} = \text{VaR}_{\mathbb{P}_n}^\alpha \{ \sqrt{n}[H(\theta) - H(\theta^c)] \},$$



which, by first-order Taylor expansion, is equal to

$$\text{VaR}_{\mathbb{P}_n}^\alpha \{X_n(\theta) + e(\theta) \|\sqrt{n}(\theta - \theta^c)\|\},$$

where  $X_n(\theta) := \nabla H(\theta^c)^\top [\sqrt{n}(\theta - \theta^c)]$  and  $e(\theta) \rightarrow 0$  if  $\theta \rightarrow \theta^c$ . Let  $\mathbb{P}_{X_n} := \mathbb{P}_n \circ X_n^{-1}$ . To show (2.3.7), we fix a  $\delta > 0$  and an  $\epsilon > 0$ . Note that since  $Y_n$  is a normal random variable, there exists an  $\eta \in (0, \min\{\alpha, 1 - \alpha\})$  such that for all  $n$ ,

$$|\text{VaR}^\alpha(Y_n) - \text{VaR}^{\alpha'}(Y_n)| = \sigma |\Phi^{-1}(\alpha) - \Phi^{-1}(\alpha')| < \delta/3 \quad \text{for} \quad \alpha' = \alpha \pm \eta. \quad (2.3.8)$$

The rest of the proof is based on constructing the following events.

- (i) By the assumption stated in Theorem 2.3.2, we can find an event  $E_1 \in \mathbb{B}_{\Xi}^{\mathbb{N}}$  with  $\mathbb{P}_{\theta^c}^{\mathbb{N}}(E_1) = 1$  such that on  $E_1$ , if  $\theta \sim \mathbb{P}_n$ , then both  $\sqrt{n}(\theta - \theta^c)$  and  $\sqrt{n}[H(\theta) - H(\theta^c)]$  have positive densities for all  $n$ .
- (ii) Since  $\mathbb{E}_{\mathbb{P}_n}[\|\sqrt{n}(\theta - \theta^c)\|]$  is bounded in probability ( $\mathbb{P}_{\theta^c}^{\mathbb{N}}$ ) by Assumption 2.3.1, there exists  $M_\epsilon > 0$  such that

$$\mathbb{P}_{\theta^c}^{\mathbb{N}} \{ \mathbb{E}_{\mathbb{P}_n}[\|\sqrt{n}(\theta - \theta^c)\|] > M_\epsilon \} < \epsilon/3, \quad \forall n.$$

Let  $E_{2,n} := \{ \mathbb{E}_{\mathbb{P}_n}[\|\sqrt{n}(\theta - \theta^c)\|] \leq M_\epsilon \}$ . There exists  $M_1 > 0$  on  $E_{2,n}$  such that

$$\mathbb{P}_n(\|\sqrt{n}(\theta - \theta^c)\| > M_1) < \eta/2, \quad \forall n \quad (2.3.9)$$

by Markov's inequality. In addition, from the strong consistency of  $\mathbb{P}_n$  and the continuity of  $e(\cdot)$ , we have

$$\mathbb{P}_n \{ |e(\theta)| > \delta/(3M_1) \} \rightarrow 0 \quad \text{in probability } (\mathbb{P}_\theta^{\mathbb{N}}).$$

Therefore, there exists  $N_1 > 0$  such that

$$\mathbb{P}_{\theta^c}^{\mathbb{N}} \{ \mathbb{P}_n(|e(\theta)| > \delta/(3M_1)) < \eta/2 \} \geq 1 - \epsilon/3, \quad \forall n > N_1. \quad (2.3.10)$$

(iii) Define  $E_{3,n} := \{ \mathbb{P}_n(|e(\theta)| > \delta/(3M_1)) < \eta/2 \}$  as in the LHS of (2.3.10). Then, on event  $E_{2,n} \cap E_{3,n}$ , we have by (2.3.9) that

$$\begin{aligned} & \mathbb{P}_n(|e(\theta)| \cdot \|\sqrt{n}(\theta - \theta^c)\| > \delta/3) \\ & \leq \mathbb{P}_n(\{|e(\theta)| > \delta/(3M_1)\} \cup \{\|\sqrt{n}(\theta - \theta^c)\| > M_1\}) < \frac{\eta}{2} + \frac{\eta}{2} = \eta \end{aligned} \quad (2.3.11)$$

for all  $n > N_1$ .

(iv) By Lemma 2.3.5 and the continuity of  $\Phi^{-1}$ , we can find  $\epsilon_1 > 0$  such that on  $E_1$ , if

$$\|\mathbb{P}_{X_n} - \mathbb{P}_{Y_n}\|_{\text{TV}} \leq \epsilon_1, \text{ then}$$

$$|\text{VaR}_{\mathbb{P}_n}^{\alpha'}(X_n(\theta)) - \text{VaR}^{\alpha'}(Y_n)| < \delta/3 \quad \text{for} \quad \alpha' = \alpha \pm \eta. \quad (2.3.12)$$

Meanwhile, since  $\|\mathbb{P}_{X_n} - \mathbb{P}_{Y_n}\|_{\text{TV}} \rightarrow 0$  in probability ( $\mathbb{P}_{\theta^c}^{\mathbb{N}}$ ) by Lemma 2.3.4, there exists  $N_2 > 0$  such that for the event  $E_{4,n} := \{\|\mathbb{P}_{X_n} - \mathbb{P}_{Y_n}\|_{\text{TV}} \leq \epsilon_1\}$ ,  $\mathbb{P}_{\theta^c}^{\mathbb{N}}(E_{4,n}) \geq 1 - \epsilon/3$  for all  $n > N_2$ .

Now consider the event  $E_n := E_1 \cap E_{2,n} \cap E_{3,n} \cap E_{4,n}$ . Take  $N := \max\{N_1, N_2\}$ . By a union bound we have  $\mathbb{P}_{\theta}^{\mathbb{N}}(E_n) \geq 1 - \epsilon/3 - \epsilon/3 - \epsilon/3 = 1 - \epsilon$  for all  $n > N$ . Moreover, on  $E_n$  we have by the definition of  $E_1$ , (2.3.11) and Lemma 2.3.3 that,

$$\text{VaR}_{\mathbb{P}_n}^{\alpha-\eta}(X_n(\theta)) - \frac{\delta}{3} \leq \text{VaR}_{\mathbb{P}_n}^{\alpha} \{ \sqrt{n}[H(\theta) - H(\theta^c)] \} \leq \text{VaR}_{\mathbb{P}_n}^{\alpha+\eta}(X_n(\theta)) + \frac{\delta}{3},$$

where by (2.3.12),

$$\text{VaR}^{\alpha-\eta}(Y_n) - \frac{2\delta}{3} \leq \text{VaR}_{\mathbb{P}_n}^{\alpha} \{ \sqrt{n}[H(\theta) - H(\theta^c)] \} \leq \text{VaR}^{\alpha+\eta}(Y_n) + \frac{2\delta}{3},$$

and finally by (2.3.8),

$$\text{VaR}^\alpha(Y_n) - \delta \leq \text{VaR}_{\mathbb{P}_n}^\alpha \left\{ \sqrt{n}[H(\theta) - H(\theta^c)] \right\} \leq \text{VaR}^\alpha(Y_n) + \delta,$$

which holds for all  $n > N$ . So (2.3.7) is proved. The conclusion follows from the fact that  $\text{VaR}^\alpha(Y_n) = \nabla H(\theta^c)^\top \Delta_n + \sigma \Phi^{-1}(\alpha)$  and  $\Delta_n \Rightarrow \mathcal{N}(0, [I(\theta^c)]^{-1})$ .  $\square$

**Remark 2.3.3.** *Since VaR is not a linear functional of random variables, the remainder term in the Taylor expansion cannot be taken directly outside VaR. Instead, we use Lemma 2.3.3 to control the error caused by ignoring the remainder term.*

**Remark 2.3.4.** *Although VaR is not uniformly continuous relative to the total variation metric, the limiting distribution  $\mathcal{N}(\Delta_n, [I(\theta^c)]^{-1})$  only varies due to  $\Delta_n$ , which is a location parameter. This allows us to show in Lemma 2.3.5 that convergence in total variation distance does imply convergence of VaR in the current situation.*

The proof for VaR demonstrates the importance and effectiveness of exploiting the structure of the limiting distribution  $\mathcal{N}(\Delta_n, [I(\theta^c)]^{-1})$ . In the upcoming proof for CVaR, we continue such exploitation by observing the following properties.

**Lemma 2.3.6.** *Suppose  $X_n \sim \mathcal{N}(c_n, \sigma^2)$  and there is a constant  $C > 0$  such that  $|c_n| < C$  for all  $n$ . Then for any  $\epsilon > 0$ , there exists  $M_{C,\epsilon} > 0$  such that*

$$\mathbb{E} \left[ |X_n| \mathbb{1}_{\{|X_n| > M_{C,\epsilon}\}} \right] < \epsilon, \quad \forall n.$$

*Proof.* Let  $Z \sim \mathcal{N}(C, \sigma^2)$ , then there exists  $M > 0$  such that  $\mathbb{E}[Z \mathbb{1}_{\{Z > M\}}] < \epsilon/2$ . It can be verified that this  $M$  corresponds to the  $\epsilon$  in the lemma.  $\square$

**Lemma 2.3.7.** *Suppose  $X_n \sim \mathcal{N}(c_n, \sigma^2)$  and there is a constant  $C > 0$  such that  $|c_n| < C$  for all  $n$ . Then for a fixed  $\alpha \in (0, 1)$  and for any  $\epsilon > 0$ , there exists  $\delta_C > 0$  such that*

$$\mathbb{E} \left[ |X_n| \mathbb{1}_{\{v_x^n - \delta_C \leq X_n \leq v_x^n + \delta_C\}} \right] < \epsilon, \quad \forall n,$$

where  $v_x^n := \text{VaR}^\alpha(X_n)$ .

*Proof.* Let  $Y \sim \mathcal{N}(0, \sigma^2)$  and write  $v_y := \text{VaR}^\alpha(Y)$  for short. Then, for a given  $\epsilon > 0$ , there exists  $\delta > 0$  such that

$$\mathbb{E} [ |Y| \mathbb{1}_{\{v_y - \delta \leq Y \leq v_y + \delta\}} ] < \frac{\epsilon}{2}.$$

Now make  $\delta$  smaller (if necessary) such that

$$\mathbb{P}(v_y - \delta \leq Y \leq v_y + \delta) < \frac{\epsilon}{2C}.$$

It can be verified that this  $\delta$  corresponds to the  $\epsilon$  in the lemma. □

**Theorem 2.3.3.** *Let Assumptions 2.2.1 and 2.3.1 hold, and  $H$  is differentiable at  $\theta^c$ . Also assume for  $\theta \sim \mathbb{P}_n$  that  $\sqrt{n}(\theta - \theta^c)$  and  $\sqrt{n}[H(\theta) - H(\theta^c)]$  have positive densities for all  $n$  a.s.  $(\mathbb{P}_{\theta^c}^{\mathbb{N}})$ . Then for any  $\alpha \in (0, 1)$ ,*

$$\sqrt{n} \{ \text{CVaR}_{\mathbb{P}_n}^\alpha [H(\theta)] - H(\theta^c) \} \Rightarrow \mathcal{N} \left( \frac{\sigma}{1 - \alpha} \phi(\Phi^{-1}(\alpha)), \sigma_x^2 \right).$$

*Proof.* Write  $\sigma_x^2$  as  $\sigma^2$  for short. Let  $X_n(\theta) := \nabla H(\theta^c)^\top [\sqrt{n}(\theta - \theta^c)]$ ,  $\mathbb{P}_{X_n} := \mathbb{P}_n \circ X_n^{-1}$ , and let  $Y_n$  denote a random variable with distribution  $\mathcal{N}(\nabla H(\theta^c)^\top \Delta_n, \sigma^2)$ . Also let  $v_x^n := \text{VaR}_{\mathbb{P}_n}^\alpha(X_n(\theta))$  and  $v_y^n := \text{VaR}^\alpha(Y_n)$ . Note that CVaR is positive homogeneous and translation invariant. By Taylor expansion,

$$\begin{aligned} & | \text{CVaR}_{\mathbb{P}_n}^\alpha \{ \sqrt{n}[H(\theta) - H(\theta^c)] \} - \text{CVaR}_{\mathbb{P}_n}^\alpha(X_n(\theta)) | \\ & \leq \text{CVaR}_{\mathbb{P}_n}^\alpha [ |e(\theta)| \cdot \|\sqrt{n}(\theta - \theta^c)\| ] \leq \frac{1}{1 - \alpha} \mathbb{E}_{\mathbb{P}_n} [ |e(\theta)| \cdot \|\sqrt{n}(\theta - \theta^c)\| ], \end{aligned}$$

which  $\Rightarrow 0$  from the proof of Theorem 2.3.1. So it suffices to show that

$$\text{CVaR}_{\mathbb{P}_n}^\alpha(X_n(\theta)) - \text{CVaR}^\alpha(Y_n) \rightarrow 0 \quad \text{in probability } (\mathbb{P}_{\theta^c}^{\mathbb{N}}).$$

Fixing a  $\delta > 0$  and an  $\epsilon > 0$ , we proceed by constructing the following events.

- (i) Since  $\mathbb{E}[Y_n] = \Delta_n$  converges in distribution, it is bounded in probability ( $\mathbb{P}_{\theta^c}^{\mathbb{N}}$ ), and thus for  $\epsilon > 0$ , there exists  $M_1 > 0$  such that for the event

$$E_{1,n} := \{|\mathbb{E}[Y_n]| \leq M_1\},$$

$\mathbb{P}_{\theta^c}^{\mathbb{N}}(E_{1,n}) > 1 - \epsilon/4$  for all  $n$ . By Lemma 2.3.7, on  $E_{1,n}$  we have for  $\delta > 0$ , there exists  $\delta_{M_1} > 0$  such that

$$\mathbb{E} \left[ |Y_n| \mathbb{1}_{\{v_y^n - \delta_{M_1} \leq Y_n \leq v_y^n + \delta_{M_1}\}} \right] < \frac{\delta}{3}. \quad (2.3.13)$$

By Lemma 2.3.6, we can find  $M_2 > 0$  such that for all  $n$ , we have on  $E_{1,n}$  that

$$\mathbb{E} \left[ |Y_n| \mathbb{1}_{\{|Y_n| > M_2\}} \right] < \frac{\delta}{6}. \quad (2.3.14)$$

- (ii) The proof of Theorem 2.3.2 implies that  $|v_x^n - v_y^n| \rightarrow 0$  in probability ( $\mathbb{P}_{\theta^c}^{\mathbb{N}}$ ), thus we can find  $N_1 > 0$  such that the event  $E_{2,n} := \{|v_x^n - v_y^n| < \delta_{M_1}\}$  satisfies  $\mathbb{P}_{\theta^c}^{\mathbb{N}}(E_{2,n}) > 1 - \epsilon/4$  for all  $n > N_1$ .
- (iii) Furthermore, since  $\mathbb{E}_{\mathbb{P}_n} [\|\sqrt{n}(\theta - \theta^c)\|^{1+\gamma}]$  is bounded in probability ( $\mathbb{P}_{\theta^c}^{\mathbb{N}}$ ) by Assumption 2.3.1, there exists  $M_\epsilon > 0$  such that

$$\mathbb{P}_{\theta^c}^{\mathbb{N}}(\mathbb{E}_{\mathbb{P}_n} [\|\sqrt{n}(\theta - \theta^c)\|^{1+\gamma}] > M_\epsilon) < \epsilon/4, \quad \forall n.$$

Let  $E_{3,n} := \{\mathbb{E}_{\mathbb{P}_n} [\|\sqrt{n}(\theta - \theta^c)\|^{1+\gamma}] \leq M_\epsilon\}$ , then by (2.3.5) we can find  $M_3 > 0$  such that for all  $n$ , we have on  $E_{3,n}$  that

$$\mathbb{E}_{\mathbb{P}_n} [|X_n(\theta)| \mathbb{1}_{\{|X_n(\theta)| > M_3\}}] < \frac{\delta}{6}. \quad (2.3.15)$$

(iv) Since  $\|\mathbb{P}_{X_n} - \mathbb{P}_{Y_n}\|_{\text{TV}} \rightarrow 0$  in probability ( $\mathbb{P}_{\theta^c}^{\mathbb{N}}$ ) by Lemma 2.3.4, there exists  $N_2 > 0$  such that for the event  $E_{4,n} := \{\|\mathbb{P}_{X_n} - \mathbb{P}_{Y_n}\|_{\text{TV}} \leq \delta/6M\}$ , we have  $\mathbb{P}_{\theta^c}^{\mathbb{N}}(E_{4,n}) > 1 - \epsilon/4$  for all  $n > N_2$ .

Now consider  $E_n := E_{1,n} \cap E_{2,n} \cap E_{3,n} \cap E_{4,n}$ . Take  $M = \max\{M_1, M_2, M_3\}$  and  $N = \max\{N_1, N_2\}$ . By a union bound,  $\mathbb{P}_{\theta^c}^{\mathbb{N}}(E_n) \geq 1 - \epsilon$  for all  $n > N$ . Assume without loss of generality that  $v_x^n \geq v_y^n$ . Then on  $E_n$ ,

$$\begin{aligned} & \left| \mathbb{E}_{\mathbb{P}_n} [X_n(\theta) \mathbb{1}_{\{X_n(\theta) \geq v_x^n\}}] - \mathbb{E} [Y_n \mathbb{1}_{\{Y_n \geq v_y^n\}}] \right| \\ & \leq \underbrace{\left| \mathbb{E}_{\mathbb{P}_n} [X_n(\theta) \mathbb{1}_{\{X_n(\theta) \geq v_x^n\}}] - \mathbb{E} [Y_n \mathbb{1}_{\{Y_n \geq v_x^n\}}] \right|}_{(*)} + \underbrace{\left| \mathbb{E} [Y_n \mathbb{1}_{\{v_y^n \leq Y_n < v_x^n\}}] \right|}_{(**)}. \end{aligned}$$

Note that since  $|v_x^n - v_y^n| < \delta_{M_1}$ ,  $(**) \leq \delta/3$  by (2.3.13). Further increase  $M$  if necessary so that  $M \geq v_x^n$ , and for  $(*)$  we have

$$\begin{aligned} \mathbb{E}_{\mathbb{P}_n} [X_n(\theta) \mathbb{1}_{\{X_n(\theta) \geq v_x^n\}}] &= \underbrace{\mathbb{E}_{\mathbb{P}_n} [X_n(\theta) \mathbb{1}_{\{X_n(\theta) > M\}}]}_{(\dagger)} + \underbrace{\mathbb{E}_{\mathbb{P}_n} [X_n(\theta) \mathbb{1}_{\{v_x^n \leq X_n(\theta) \leq M\}}]}_{(***)}, \\ \mathbb{E} [Y_n \mathbb{1}_{\{Y_n \geq v_x^n\}}] &= \underbrace{\mathbb{E} [Y_n \mathbb{1}_{\{Y_n > M\}}]}_{(\dagger\dagger)} + \underbrace{\mathbb{E} [Y_n \mathbb{1}_{\{v_x^n \leq Y_n \leq M\}}]}_{(****)}, \end{aligned}$$

where  $|(\dagger)| < \delta/6$  by (2.3.15) and  $|(\dagger\dagger)| < \delta/6$  by (2.3.14). Define  $X^+ := \max(X, 0)$  and  $X^- := -\min(X, 0)$ , and we have

$$\begin{aligned} (* *) &= \mathbb{E}_{\mathbb{P}_n} [X_n^+(\theta) \mathbb{1}_{\{v_x^n \leq X_n(\theta) \leq M\}}] - \mathbb{E}_{\mathbb{P}_n} [X_n^-(\theta) \mathbb{1}_{\{v_x^n \leq X_n(\theta) \leq M\}}] \\ &= \int_0^\infty \mathbb{P}_n (X_n^+(\theta) \mathbb{1}_{\{v_x^n \leq X_n(\theta) \leq M\}} > t) dt - \int_0^\infty \mathbb{P}_n (X_n^-(\theta) \mathbb{1}_{\{v_x^n \leq X_n(\theta) \leq M\}} > t) dt \\ &= \int_0^M \mathbb{P}_n (v_x^n \leq X_n(\theta) \leq M, X_n(\theta) > t) dt \\ &\quad - \int_0^M \mathbb{P}_n (v_x^n \leq X_n(\theta) \leq M, X_n(\theta) < -t) dt, \end{aligned}$$

and similarly,  $(***)$  can be expressed by

$$\int_0^M \mathbb{P}(v_x^n \leq Y_n \leq M, Y_n > t) dt - \int_0^M \mathbb{P}(v_x^n \leq Y_n \leq M, Y_n < -t) dt.$$

It follows from  $\|\mathbb{P}_{X_n} - \mathbb{P}_{Y_n}\|_{\text{TV}} \leq \delta/6M$  that

$$|(**) - (***)| \leq M \frac{\delta}{6M} + M \frac{\delta}{6M} = \frac{\delta}{3}.$$

In sum, we have

$$(*) + (**) \leq \frac{\delta}{6} + \frac{\delta}{6} + \frac{\delta}{3} + \frac{\delta}{3} = \delta,$$

thus,

$$\mathbb{P}_{\theta^c}^{\mathbb{N}} \left\{ \left| \mathbb{E}_{\mathbb{P}_n} [X_n(\theta) \mathbb{1}_{\{X_n(\theta) \geq v_x^n\}}] - \mathbb{E} [Y_n \mathbb{1}_{\{Y_n \geq v_y^n\}}] \right| \leq \delta \right\} \geq 1 - \epsilon, \quad \forall n > N,$$

which implies that  $\text{CVaR}_{\mathbb{P}_n}^{\alpha}(X_n(\theta)) - \text{CVaR}^{\alpha}(Y_n) \rightarrow 0$  in probability  $(\mathbb{P}_{\theta^c}^{\mathbb{N}})$ . We now conclude that

$$\text{CVaR}_{\mathbb{P}_n}^{\alpha} \{ \sqrt{n} [H(\theta) - H(\theta^c)] \} - \text{CVaR}^{\alpha}(Y_n) \rightarrow 0 \text{ in probability } (\mathbb{P}_{\theta^c}^{\mathbb{N}}).$$

But

$$\text{CVaR}^{\alpha}(Y_n) = \nabla H(\theta^c)^{\top} \Delta_n + \frac{\sigma}{1-\alpha} \phi(\Phi^{-1}(\alpha)) \Rightarrow \mathcal{N} \left( \frac{\sigma}{1-\alpha} \phi(\Phi^{-1}(\alpha)), \sigma^2 \right),$$

so the proof is complete. □

**Remark 2.3.5.** *Our proof for CVaR relies on the proof for VaR (see the construction of  $E_{2,n}$ ). Moreover, from the construction of  $E_{3,n}$  and (2.3.15) we see that Assumption 2.3.1 is critical to bounding the truncated tail expectation of  $X_n(\theta)$ . This is not surprising since Assumption 2.3.1 essentially characterizes a form of uniform integrability, which is a well-*

known sufficient condition for bridging the gap between convergence in total variation (or weak convergence) and convergence of expectations.

### 2.3.2 Asymptotic Normality of Optimal Values.

The goal of this section is to establish asymptotic normality of the optimal values

$$\sqrt{n} \left( \min_{x \in \mathcal{X}} \rho_{\mathbb{P}_n} [H(x, \theta)] - \min_{x \in \mathcal{X}} H(x, \theta^c) \right). \quad (2.3.16)$$

Let  $C(\mathcal{X})$  denote the Banach space of all continuous functions on a compact set  $\mathcal{X}$  equipped with the sup-norm. Also let  $\mathcal{C}_{\mathcal{X}}$  denote the Borel  $\sigma$ -algebra on  $C(\mathcal{X})$ . A random element <sup>4</sup> is defined as a mapping from  $(\Omega, \mathcal{F})$  to  $(C(\mathcal{X}), \mathcal{C}_{\mathcal{X}})$ , i.e., each realization of a random element is a continuous function in  $C(\mathcal{X})$ . Definition 2.2.1 of weak convergence carries over to this space, except that one need to consider all bounded and continuous functionals on  $C(\mathcal{X})$ . In words, for  $f_n, f \in C(\mathcal{X})$ ,  $f_n \Rightarrow f$  characterizes the weak convergence of continuous random functions. Define

$$g_n(x) := \sqrt{n} \{ \rho_{\mathbb{P}_n} [H(x, \theta)] - H(x, \theta^c) \}.$$

To study the asymptotic distribution of (2.3.16), we will resort to the following result.

**Lemma 2.3.8** (Theorem 3.2 in [25]). *If  $\sqrt{n}(f_n - \bar{f}) \Rightarrow Y_x$ , where  $f_n, \bar{f}$  and  $Y_x$  are random elements of  $C(\mathcal{X})$ , then*

$$\sqrt{n} \left( \min_{x \in \mathcal{X}} f_n - \min_{x \in \mathcal{X}} \bar{f} \right) \Rightarrow \min_{x \in S} Y_x \quad \text{as } n \rightarrow \infty, \quad (2.3.17)$$

where  $S := \arg \min_{x \in \mathcal{X}} \bar{f}$ .

To apply (2.3.8), we need to show that (i)  $\rho_{\mathbb{P}_n} [H(\cdot, \theta)]$  and  $H(\cdot, \theta^c)$  are continuous

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<sup>4</sup>A random element is a generalization of the concept of random variable to more complicated spaces than  $\mathbb{R}$ .



functions on  $\mathcal{X}$ ; (ii)  $g_n(\cdot)$  converges weakly to some random element of  $C(\mathcal{X})$ . In many applications involving empirical distributions (e.g., [26, 27]), results similar to (ii) can be established using a functional Central Limit Theorem. However, this is not applicable to the Bayesian setting considered in this chapter. Instead, we will prove (ii) via two steps. First, we show the weak convergence of  $g_n$ 's finite-dimensional distributions, i.e., the weak convergence of

$$[g_n(x_1), g_n(x_2), \dots, g_n(x_k)]$$

for any finite sequence  $x_1, x_2, \dots, x_k \in \mathcal{X}$ . Then, by Theorem 7.5 in [73], the weak convergence of  $g_n$  can be established by checking the following condition

$$\lim_{\delta \rightarrow 0} \limsup_{n \rightarrow \infty} \mathbb{P}_{\theta^c}^{\mathbb{N}} (\zeta(g_n, \delta) \geq \epsilon) = 0, \quad \forall \epsilon > 0, \quad (2.3.18)$$

where  $\zeta(f, \delta)$  is the modulus of continuity of  $f \in C(\mathcal{X})$  and is defined as

$$\zeta(f, \delta) := \sup_{\substack{\|x - x'\| < \delta \\ x, x' \in \mathcal{X}}} |f(x) - f(x')|. \quad (2.3.19)$$

The condition in (2.3.18) is also known as stochastic equicontinuity (s.e.). It guarantees the tightness of  $g_n$ 's distributions, which implies weak convergence essentially due to the Arzelà-Ascoli Theorem (see, e.g., [73, Theorem 7.2]). For more details on weak convergence in the  $C$  space, we refer the reader to [73, Section 7].

**Theorem 2.3.4.** *Suppose that Assumptions 2.2.1 and 2.3.1 hold. Also assume for  $\theta \sim \mathbb{P}_n$  that  $\sqrt{n}(\theta - \theta^c)$  and  $\sqrt{n}[H(\theta) - H(\theta^c)]$  have positive densities for all  $n$  a.s. ( $\mathbb{P}_{\theta^c}^{\mathbb{N}}$ ). Further suppose  $\mathcal{X}$  is a compact set,  $H$  is continuous on  $\mathcal{X} \times \Theta$ , and  $H(x, \cdot)$  differentiable at  $\theta^c$  for all  $x \in \mathcal{X}$ , where  $\nabla_{\theta} H(\cdot, \theta^c)$  is continuous on  $\mathcal{X}$ . Then,*

$$\sqrt{n} \left( \min_{x \in \mathcal{X}} \rho_{\mathbb{P}_n} [H(x, \theta)] - \min_{x \in \mathcal{X}} H(x, \theta^c) \right) \Rightarrow \min_{x \in S} Y_x,$$

where  $S := \arg \min_{x \in \mathcal{X}} H(x, \theta^c)$  and

$$Y_x := \begin{cases} \nabla_{\theta} H(x, \theta^c)^{\top} Z & \text{if } \rho = \text{mean} / \text{mean-variance} \\ \nabla_{\theta} H(x, \theta^c)^{\top} Z + \sigma_x \Phi^{-1}(\alpha) & \text{if } \rho = \text{VaR} \\ \nabla_{\theta} H(x, \theta^c)^{\top} Z + \frac{\phi(\Phi^{-1}(\alpha))}{1-\alpha} \sigma_x & \text{if } \rho = \text{CVaR} \end{cases},$$

where  $Z$  is a random variable following distribution  $\mathcal{N}(0, [I(\theta^c)]^{-1})$ .

**Proof. Step 1.** Since  $\mathcal{X} \times \Theta$  is compact by the Tychonoff Product Theorem (see, e.g., [76, Page 245]),  $H$  is uniformly continuous on  $\mathcal{X} \times \Theta$  by the Heine-Cantor Theorem (see, e.g., [77, Theorem 4.19]). Thus, for any  $\epsilon > 0$ , there exists  $\delta > 0$  such that  $|H(x, \theta) - H(x', \theta')| < \epsilon$  as long as  $\|(x, \theta) - (x', \theta')\| < \delta$ . For the mean, VaR and CVaR formulations, if  $\|(x, \theta) - (x', \theta)\| = \|x - x'\| < \delta$ , then by Lemma 2.2.5,

$$|\rho_{\mathbb{P}_n}\{H(x, \theta)\} - \rho_{\mathbb{P}_n}\{H(x', \theta)\}| \leq \sup_{\theta \in \Theta} |H(x, \theta) - H(x', \theta)| < \epsilon.$$

So  $\rho_{\mathbb{P}_n}\{H(\cdot, \theta)\}$  is uniformly continuous on  $\mathcal{X}$  for mean, VaR and CVaR. The case of mean-variance follows from the continuity of  $H^2$  on  $\mathcal{X} \times \Theta$ .

**Step 2.** The next step is to show the weak convergence of finite-dimensional distributions. Since mean, VaR and CVaR are linear functionals, we have

$$g_n(x) = \rho_{\mathbb{P}_n} \left\{ \sqrt{n} [H(x, \theta) - H(x, \theta^c)] \right\}.$$

Fix a finite sequence  $x_1, x_2, \dots, x_k \in \mathcal{X}$ . For  $[g_n(x_1), g_n(x_2), \dots, g_n(x_k)]$ , we apply Taylor expansion inside the functional  $\rho$  for each dimension. The remainder terms also form a  $k$ -dimensional random vector, which converges in probability to 0 if and only if each dimension does. Thus, the proofs of Theorems 2.3.1, 2.3.2, and 2.3.3 can be easily extended to show that each formulation's finite-dimensional distributions converge weakly to that of  $Y_x$  defined in the statement of Theorem 2.3.4.

**Step 3.** By [73, Theorem 7.5], the proof will be complete if we show that  $g_n(\cdot)$  is s.e. (defined as in (2.3.18)) for all four choices of  $\rho$ , where the specific forms of  $Y_x$  follows from Theorems 2.3.1, 2.3.2 and 2.3.3. We now prove s.e. for each choice of  $\rho$ .

(i) Mean formulation: By Taylor expansion,

$$g_n(x) = \nabla_{\theta} H(x, \theta^c)^{\top} \mathbb{E}_{\mathbb{P}_n} [\sqrt{n}(\theta - \theta^c)] + \mathbb{E}_{\mathbb{P}_n} [e(x, \theta) \|\sqrt{n}(\theta - \theta^c)\|],$$

where it suffices to show s.e. for the two terms in the RHS. Since  $\mathbb{E}_{\mathbb{P}_n} [\sqrt{n}(\theta - \theta^c)]$  converges weakly by Assumption 2.3.1, for any  $\eta > 0$ , there exists  $M_{\eta} > 0$  such that

$$\mathbb{P}_{\theta^c}^{\mathbb{N}}(\|\mathbb{E}_{\mathbb{P}_n} [\sqrt{n}(\theta - \theta^c)]\| < M_{\eta}) > 1 - \eta, \quad \forall n.$$

Since we assume that  $\nabla_{\theta} H(\cdot, \theta^c)$  is continuous (and hence uniformly continuous) on  $\mathcal{X}$ , for any  $\epsilon > 0$ , there exists  $\delta_{\eta} > 0$  such that

$$\sup_{\substack{\|x - x'\| < \delta_{\eta} \\ x, x' \in \mathcal{X}}} \|\nabla_{\theta} H(x, \theta^c) - \nabla_{\theta} H(x', \theta^c)\| < \epsilon/M_{\eta}.$$

It follows that on the event  $\{\|\mathbb{E}_{\mathbb{P}_n} [\sqrt{n}(\theta - \theta^c)]\| < M_{\eta}\}$ , we have

$$\zeta(\nabla_{\theta} H(x, \theta^c)^{\top} \mathbb{E}_{\mathbb{P}_n} [\sqrt{n}(\theta - \theta^c)], \delta_{\eta}) < \frac{\epsilon}{M_{\eta}} M_{\eta} = \epsilon,$$

where  $\zeta$  is the modulus of continuity defined in (2.3.19). Therefore, the first term has the s.e. property. For the second term, we only need to show that

$$\sup_{x \in \mathcal{X}} |\mathbb{E}_{\mathbb{P}_n} [e(x, \theta) \|\sqrt{n}(\theta - \theta^c)\|]| \Rightarrow 0.$$

Since

$$\sup_{x \in \mathcal{X}} |\mathbb{E}_{\mathbb{P}_n}[e(x, \theta) \|\sqrt{n}(\theta - \theta^c)\|]| \leq \mathbb{E}_{\mathbb{P}_n} \left[ \sup_{x \in \mathcal{X}} |e(x, \theta)| \|\sqrt{n}(\theta - \theta^c)\| \right],$$

it suffices to show for  $\theta \sim \mathbb{P}_n$  that  $\sup_{x \in \mathcal{X}} |e(x, \theta)| \Rightarrow 0$  a.s.  $(\mathbb{P}_{\theta^c}^{\mathbb{N}})$ . However, the continuity of  $e$  on  $\mathcal{X} \times \Theta$  implies that  $\sup_{x \in \mathcal{X}} |e(x, \cdot)|$  is continuous on  $\Theta$ . Setting  $e(x, \theta^c) = 0$  for all  $x \in \mathcal{X}$  does not affect the Taylor expansion, so for  $\theta \sim \mathbb{P}_n$ ,

$$\sup_{x \in \mathcal{X}} |e(x, \theta)| \Rightarrow \sup_{x \in \mathcal{X}} |e(x, \theta^c)| = 0 \quad \text{a.s. } (\mathbb{P}_{\theta^c}^{\mathbb{N}}),$$

and the rest follows from the proof of Theorem 2.3.1.

(ii) Mean-variance formulation: Since  $\nabla_{\theta} H(\cdot, \theta^c)$  is bounded on  $\mathcal{X}$  and  $e$  is bounded on  $\mathcal{X} \times \Theta$ , it follows from the proof of Theorem 2.3.1 that

$$\sup_{x \in \mathcal{X}} \sqrt{n} \text{Var}_{\mathbb{P}_n}[H(x, \theta)] \Rightarrow 0,$$

which implies the s.e. for mean-variance.

(iii) VaR formulation: Recall that the proof of Theorem 2.3.2 is based on bounding

$$(\dagger) = g_n(x) - \text{VaR}_{\mathbb{P}_n}^{\alpha \pm \epsilon_1} \{ \nabla_{\theta} H(x, \theta^c)^{\top} [\sqrt{n}(\theta - \theta^c)] \},$$

by (2.3.11) and Lemma 2.3.3 for some  $\epsilon_1 > 0$ , and

$$(\dagger\dagger) = \text{VaR}_{\mathbb{P}_n}^{\alpha \pm \epsilon_1} \{ \nabla_{\theta} H(x, \theta^c)^{\top} [\sqrt{n}(\theta - \theta^c)] \} - \text{VaR}_{\mathbb{P}_n}^{\alpha \pm \epsilon_1} \{ \mathcal{N}(\nabla H(x, \theta^c)^{\top} \Delta_n, \sigma_x^2) \},$$

by (2.3.12), where the bound on  $|(\dagger)|$  depends on  $x$  via  $e(x, \theta)$ , and the bound on  $|(\dagger\dagger)|$  does not depend on  $x$  due to Lemma 2.3.4. Since we have for  $\theta \sim \mathbb{P}_n$  that  $\sup_{x \in \mathcal{X}} |e(x, \theta)| \Rightarrow 0$

a.s.  $(\mathbb{P}_{\theta^c}^{\mathbb{N}})$ , following the proof of Theorem 2.3.2 yields that

$$\sup_{x \in \mathcal{X}} |g_n(x) - \text{VaR}_{\mathbb{P}_n}^{\alpha} \{ \mathcal{N}(\nabla H(x, \theta^c)^{\top} \Delta_n, \sigma_x^2) \}| \rightarrow 0 \quad \text{in probability } (\mathbb{P}_{\theta^c}^{\mathbb{N}}).$$

But we know

$$\text{VaR}^{\alpha} \{ \mathcal{N}(\nabla H(x, \theta^c)^{\top} \Delta_n, \sigma_x^2) \} = \nabla_{\theta} H(x, \theta^c)^{\top} \Delta_n + \sigma_x \Phi^{-1}(\alpha)$$

has s.e. since  $\nabla_{\theta} H(\cdot, \theta^c)$  and  $\sigma_x^2$  are uniformly continuous on  $\mathcal{X}$  and  $\Delta_n$  converges in distribution. So the case of VaR is proved.

(iv) CVaR formulation: Since

$$g_n(x) = \text{CVaR}_{\mathbb{P}_n}^{\alpha} \{ \nabla_{\theta} H(x, \theta^c)^{\top} [\sqrt{n}(\theta - \theta^c)] + e(x, \theta) \|\sqrt{n}(\theta - \theta^c)\| \},$$

we have

$$\begin{aligned} \zeta(g_n, \delta) \leq & \sup_{\substack{\|x - x'\| < \delta \\ x, x' \in \mathcal{X}}} \frac{1}{1 - \alpha} \{ \mathbb{E}_{\mathbb{P}_n} [ \|\nabla_{\theta} H(x, \theta^c) - \nabla_{\theta} H(x', \theta^c)\| \|\sqrt{n}(\theta - \theta^c)\| ] \\ & + \mathbb{E}_{\mathbb{P}_n} [ |e(x, \theta) - e(x', \theta)| \|\sqrt{n}(\theta - \theta^c)\| ] \}, \end{aligned}$$

and the rest follows from the proof for mean. □

## 2.4 Interpretation of Bayesian risk optimization

We now interpret BRO based on the asymptotic normality results established in Section 2.3.2. Following the notations in Theorem 2.3.4, let  $Z$  denote a random variable with distribution  $\mathcal{N}(0, [I(\theta^c)]^{-1})$ . We write  $\sigma_x$  as  $\sigma(\cdot)$  to emphasize that it is a function of  $x$ . Taking the VaR formulation as an example, from the proof of Theorem 2.3.4 (for VaR) we

have the following weak convergence result in the  $C$  space.

$$\sqrt{n} \{ \text{VaR}_{\mathbb{P}_n}^\alpha [H(\cdot, \theta)] - H(\cdot, \theta^c) \} \Rightarrow \nabla_\theta H(\cdot, \theta^c)^\top Z + \Phi^{-1}(\alpha) \sigma(\cdot).$$

This can be rewritten as

$$\text{VaR}_{\mathbb{P}_n}^\alpha [H(\cdot, \theta)] \stackrel{\mathcal{D}}{=} H(\cdot, \theta^c) + \frac{\nabla_\theta H(\cdot, \theta^c)^\top Z}{\sqrt{n}} + \Phi^{-1}(\alpha) \frac{\sigma(\cdot)}{\sqrt{n}} + o_p\left(\frac{1}{\sqrt{n}}\right), \quad (2.4.1)$$

where “ $\stackrel{\mathcal{D}}{=}$ ” means “is distributionally equivalent to”, and  $o_p(1/\sqrt{n})$  stands for a term whose product with  $\sqrt{n}$  converges to 0 in probability ( $\mathbb{P}_{\theta^c}^\mathbb{N}$ ) uniformly in  $x$ . The LHS of (2.4.1) is the VaR objective we propose to minimize, and the RHS can be viewed as the sum of the true objective  $H(\cdot, \theta^c)$  and some error terms. Compared with the mean formulation, whose objective can be written as

$$\mathbb{E}_{\mathbb{P}_n} [H(\cdot, \theta)] \stackrel{\mathcal{D}}{=} H(\cdot, \theta^c) + \frac{\nabla_\theta H(\cdot, \theta^c)^\top Z}{\sqrt{n}} + o_p\left(\frac{1}{\sqrt{n}}\right), \quad (2.4.2)$$

we see that (2.4.1) has an extra deterministic bias term  $\Phi^{-1}(\alpha) \sigma(\cdot)/\sqrt{n}$  that vanishes as  $n \rightarrow \infty$ . Combining (2.4.1) and (2.4.2), we have

$$\text{VaR}_{\mathbb{P}_n}^\alpha [H(\cdot, \theta)] \stackrel{\mathcal{D}}{=} \mathbb{E}_{\mathbb{P}_n} [H(\cdot, \theta)] + \Phi^{-1}(\alpha) \frac{\sigma(\cdot)}{\sqrt{n}} + o_p\left(\frac{1}{\sqrt{n}}\right).$$

Therefore, the VaR formulation’s objective approximately equals a weighted sum of posterior mean and a bias  $\sigma(\cdot)/\sqrt{n}$ , where the weight of the bias is  $\Phi^{-1}(\alpha)$ . Although the bias diminishes as  $n \rightarrow \infty$ , it has an undeniable impact on the VaR objective when  $n$  is small. In particular, if  $n$  is not too large (e.g. 20) and  $\alpha$  is close to 1 (e.g. 99%), it is possible for the bias term to dominate  $\mathbb{E}_{\mathbb{P}_n} [H(x, \theta)]$  and we are close to solving  $\min_{x \in \mathcal{X}} \sigma_x / \sqrt{n}$ .

Similarly, the CVaR objective can be rewritten as

$$\text{CVaR}_{\mathbb{P}_n}^\alpha \{H(\cdot, \theta)\} \stackrel{\mathcal{D}}{=} \mathbb{E}_{\mathbb{P}_n}[H(\cdot, \theta)] + \frac{\phi(\Phi^{-1}(\alpha))}{1 - \alpha} \frac{\sigma(\cdot)}{\sqrt{n}} + o_p\left(\frac{1}{\sqrt{n}}\right).$$

For the mean-variance formulation, by imposing appropriate conditions of uniform integrability, it can be shown that the variance satisfies

$$\text{Var}_{\mathbb{P}_n}[H(\cdot, \theta)] = \frac{1}{n} \text{Var}_{\mathbb{P}_n} \{ \sqrt{n}[H(\cdot, \theta) - H(\cdot, \theta^c)] \} \stackrel{\mathcal{D}}{=} \frac{\sigma^2(\cdot)}{n} + o_p\left(\frac{1}{n}\right).$$

Thus, the objective functions of the mean-variance, VaR and CVaR formulations are all approximately equivalent to a weighted sum of the mean objective and  $\sigma(\cdot)/\sqrt{n}$  (or  $(\sigma(\cdot)/\sqrt{n})^2$ ), where the weight of  $\sigma(\cdot)/\sqrt{n}$  is controlled by  $\alpha$  in the VaR and CVaR formulations, and the weight of  $(\sigma(\cdot)/\sqrt{n})^2$  is controlled by the constant  $w$  in the mean-variance formulation.

At this point, one naturally wonders the implication of minimizing  $\sigma(\cdot)/\sqrt{n}$ . For a fixed  $x \in \mathcal{X}$ , Theorems 2.3.1, 2.3.2 and 2.3.3 allow the following asymptotical valid  $100(1-\beta)\%$  confidence intervals (CIs) of  $H(x, \theta^c)$  (in the form of center  $\pm$  half-width).

(i) The mean and mean-variance formulation

$$(\mathbb{E}_{\mathbb{P}_n}[H(x, \theta)] + w \text{Var}_{\mathbb{P}_n}[H(x, \theta)]) \pm z_{1-\frac{\beta}{2}} \frac{\sigma_x}{\sqrt{n}},$$

(ii) The VaR formulation

$$\left( \text{VaR}_{\mathbb{P}_n}^\alpha [H(x, \theta)] - \frac{\Phi^{-1}(\alpha)\sigma_x}{\sqrt{n}} \right) \pm z_{1-\frac{\beta}{2}} \frac{\sigma_x}{\sqrt{n}},$$

(iii) The CVaR formulation

$$\left( \text{CVaR}_{\mathbb{P}_n}^\alpha [H(x, \theta)] - \frac{\phi(\Phi^{-1}(\alpha))\sigma_x}{(1 - \alpha)\sqrt{n}} \right) \pm z_{1-\frac{\beta}{2}} \frac{\sigma_x}{\sqrt{n}},$$

where  $z_{1-\beta}$  denotes the  $(1 - \beta)$ -quantile of a standard normal distribution. Observe that  $\sigma_x/\sqrt{n}$  is exactly proportional to the half-width of the CI, where narrower CI implies higher accuracy of estimating the true performance  $H(x, \theta^c)$ , while a wider CI indicates higher risk due to less confidence about how a solution actually performs. *In other words, BRO is essentially seeking a tradeoff between posterior expected performance and the robustness in actual performance.* It is also interesting to notice that  $\sigma_x$  depends on  $\nabla_\theta H(x, \theta^c)$  and  $I(\theta^c)$ , where  $\nabla_\theta H(x, \theta^c)$  is the sensitivity of the function  $H$  to the perturbation of the parameter  $\theta^c$  (i.e., IU), while  $I(\theta^c)$  is the Fisher information that captures the amount of information a data sample carries about the true parameter.

## 2.5 Conclusion and Future Work

We formally propose a framework of Bayesian risk optimization (BRO) for simulation optimization under input uncertainty, and study the implications of BRO by establishing a series of consistency and asymptotic normality results. The analysis on asymptotics leads to an important insight: BRO explicitly seeks a tradeoff between posterior mean performance and the risk in a solution's actual performance. A question of practical interest is whether our insight can be used as an approximate method to solve the BRO problem, but the mixed impact of input uncertainty and simulation uncertainty needs to be taken into account. In addition, our proofs assume compactness of the parameter space, but it is worth studying more general cases since many priors are not supported on compact sets. It is also interesting to consider a nonparametric setting with a prior of Dirichlet process, though the associated asymptotics could be much more complicated.



## CHAPTER 3

### ANALYZING AND PROVABLY IMPROVING FIXED BUDGET RANKING AND SELECTION ALGORITHMS

This chapter centers on the classical fixed budget R&S problem without input uncertainty, which can be viewed as a crucial building block for studying R&S under IU in Chapter 4. We study the well-known Optimal Computing Budget Allocation algorithm, and reveal that its popular implementation is subject to a slow convergence rate. A modification is proposed to improve its performance both theoretically and practically. Furthermore, we explicitly characterize the convergence rate of several simplified algorithms, showcasing some interesting insights and useful techniques for conducting general convergence analysis in the fixed budget setting.

The rest of the chapter is organized as follows. A brief review on the fixed budget R&S problem is provided in Section 3.1. Section 3.2 reveals the shortcoming of budget-independent initial sample size for three OCBA-type algorithms, and proposes a modification to improve their convergence rate. Section 3.3 conducts a preliminary study on convergence rate characterization by analyzing some simplified algorithms in a two-design case. Numerical results are presented in section 3.4, followed by conclusion and future work in section 3.5.

#### 3.1 Problem Formulation

Given a set of designs  $\mathcal{I} = \{1, \dots, K\}$ , our goal is to select (without loss of generality) the one with the highest expected performance. Samples from simulating design  $i$  are denoted by  $X_{ir}$ , where  $r$  denotes the  $r$ th simulation run. Each design's expected performance is unknown, and is typically evaluated through multiple simulation runs and estimated by the

sample mean

$$\bar{X}_{i,N_i} := \frac{1}{N_i} \sum_{r=1}^{N_i} X_{ir},$$

where  $N_i$  is how many times design  $i$  has been sampled/simulated. The subscript  $N_i$  will be suppressed when there is no ambiguity. The true best and the observed best designs are denoted by

$$b := \arg \max_{i \in \mathcal{I}} \mu_i, \quad \hat{b} := \arg \max_{i \in \mathcal{I}} \bar{X}_i,$$

respectively. We make the following standard assumptions to avoid technicalities, where  $\mathcal{N}$  stands for normal distribution and “i.i.d.” means “independent and identically distributed”.

**Assumption 3.1.1.**

- (i)  $K \geq 2$  and  $\mu_i \neq \mu_j$  for any two different designs  $i$  and  $j$ .
- (ii) For each design  $i$ ,  $\{X_{ir}\}$  are i.i.d. samples from  $\mathcal{N}(\mu_i, \sigma_i^2)$ , where  $\sigma_i > 0$ . The samples are also independent across different designs.

Then, under a fixed budget  $T$  of simulation runs, it is desired to maximize the probability of correct selection (PCS), which is defined as

$$\text{PCS} := \mathbb{P} \left\{ \hat{b} = b \right\} = \mathbb{P} \left\{ \bigcap_{i \neq b} \{ \bar{X}_b > \bar{X}_i \} \right\}.$$

We will also refer to  $1 - \text{PCS}$  as the probability of false selection (PFS). The challenge of fixed budget R&S problem lies in how to make the best use of a finite simulation budget to distinguish the best design from the rest. Numerous algorithms have been proposed to this end, and their performance is typically evaluated using two types of measures.

The first type is asymptotic measures, which are often based on the large deviations (LD) theory. It has been shown in [40] that many algorithms have the following asymptotic property.

$$-\lim_{T \rightarrow \infty} \frac{1}{T} \log \text{PFS}_{\mathcal{A}}(T, P) = R_{\mathcal{A}}(P), \quad (3.1.1)$$

where  $\mathcal{A}$  is an algorithm,  $P$  is a problem instance,  $\text{PFS}_{\mathcal{A}}(T, P)$  is the PFS of algorithm  $\mathcal{A}$  applied to problem  $P$  under budget  $T$ , and  $R_{\mathcal{A}}(\cdot) \geq 0$  is called an LD rate function. For convenience, we say an algorithm  $\mathcal{A}$  has an *exponential convergence rate* if its PFS converges exponentially fast to 0, i.e., its LD rate  $R_{\mathcal{A}}$  is positive. Asymptotically optimal algorithms have been derived by maximizing  $R_{\mathcal{A}}$  (see, e.g., [40]), but it is an insufficient performance measure since it focuses primarily on the asymptotic performance. For example, all the terms in  $\{e^{-T}, Te^{-T}, T^2e^{-T}, \dots\}$  have the same LD rate according to (3.1.1), yet they behave quite differently for small values of  $T$ .

Measures of the second type emphasize more on the finite-sample performance. One approach is to approximate the PFS using tight bounds, but it could be remarkably difficult for algorithms that allocate the budget in a sequential style. Another approach is to plot out the PCS curve and visualize how fast it converges to 1 as  $T$  increases. The main downside, however, is that such empirical results are problem-specific and may fail to represent the general performance of an algorithm.

Bearing the pros and cons of these three approaches in mind, we will analyze and improve existing algorithms from an LD perspective, and substantiate the improvement using finite-samples bounds combined with numerical results.

### 3.2 Analyzing and Improving OCBA-type Algorithms

This section gives a brief introduction to OCBA and two of its variants, which we call OCBA-D and OCBA-R. To better describe the algorithms, we introduce the following notations. Let  $S_{i,n}^2$  denote the standard sample variance estimator of  $n$  i.i.d. samples from design  $i$ , and let  $\ell$  denote the iteration number of the algorithms, where  $\ell = 0$  corresponds to the initialization phase. The budget allocated to design  $i$  at the end of the  $\ell$ th iteration is written as  $N_i(\ell)$ , and other quantities are defined accordingly. For example, we let  $\bar{X}_i(\ell) := \bar{X}_{i,N_i(\ell)}$  and  $S_i^2(\ell) := S_{i,N_i(\ell)}^2$ . The OCBA algorithm is presented in Algorithm 1.

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**Algorithm 1** OCBA (Chen et al. (2000))

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```
1: Input:  $N_0 \geq 2, \Delta \geq 1, T \geq KN_0$ .  
2: Initialization: Sample each design  $N_0$  times and compute  $\bar{X}_i(0)$  and  $S_i^2(0)$ .  $N_i(0) \leftarrow N_0$ .  $T'(0) \leftarrow N_0K + \Delta$ .  $\ell \leftarrow 0$ .  
3: while  $\sum_{i \in \mathcal{I}} N_i(\ell) < T$  and  $T'(\ell) \leq T$  do  
4:    $\hat{b} \leftarrow \arg \max_{i \in \mathcal{I}} \bar{X}_i(\ell)$ .  
5:   Compute  $\hat{\alpha}_1(\ell), \dots, \hat{\alpha}_K(\ell)$  using (3.2.1).  
6:   for  $i = 1, \dots, K$  do  
7:     Run  $\max\{0, \lfloor \hat{\alpha}_i(\ell)T'(\ell) \rfloor - N_i(\ell)\}$  replications for design  $i$ .  
8:      $N_i(\ell + 1) \leftarrow \max\{N_i(\ell), \lfloor \hat{\alpha}_i(\ell)T'(\ell) \rfloor\}$ . Compute  $\bar{X}_i(\ell + 1)$  and  $S_i(\ell + 1)$ .  
9:   end for  
10:   $\ell \leftarrow \ell + 1$ .  
11:   $T'(\ell + 1) \leftarrow T'(\ell) + \Delta$ .  
12: end while  
13: Output:  $\hat{b} = \arg \max_{i \in \mathcal{I}} \bar{X}_i(\ell)$ .
```

---

### 3.2.1 OCBA, OCBA-D, and OCBA-R

OCBA-D and OCBA-R. To better describe the algorithms, we introduce the following notations. Let  $S_{i,n}^2$  denote the standard sample variance estimator of  $n$  i.i.d. samples from design  $i$ , and let  $\ell$  denote the iteration number of the algorithms, where  $\ell = 0$  corresponds to the initialization phase. The budget allocated to design  $i$  at the end of the  $\ell$ th iteration is written as  $N_i(\ell)$ , and other quantities are defined accordingly. For example, we let  $\bar{X}_i(\ell) := \bar{X}_{i,N_i(\ell)}$  and  $S_i^2(\ell) := S_{i,N_i(\ell)}^2$ . The OCBA algorithm is presented in Algorithm 1.

OCBA has three input parameters: (i)  $N_0 \geq 2$  is the size of samples for an initial estimation of each design's mean and variance; (ii)  $\Delta \geq 1$  is the increment of available budget at each iteration; (iii)  $T \geq KN_0$  is the total budget. An auxiliary variable,  $T'$ , is introduced to implement sequential allocation. The procedure begins with estimating each design's mean and variance using  $N_0$  samples, where  $T'$  is set to be  $KN_0$ . Then, at each iteration, the algorithm increases  $T'$  by  $\Delta$ , and (re)computes the fractions  $\hat{\alpha}_1(\ell), \dots, \hat{\alpha}_K(\ell)$

according to the following equations.

$$\hat{\beta}_i(\ell) = \begin{cases} S_i^2(\ell)/[\bar{X}_{\hat{b}}(\ell) - \bar{X}_i(\ell)]^2 & \text{if } i \neq \hat{b} \\ S_{\hat{b}}(\ell)\sqrt{\sum_{i \neq \hat{b}} \hat{\beta}_i^2(\ell)/S_i^2(\ell)} & \text{o./w} \end{cases}, \quad \hat{\alpha}_i(\ell) := \frac{\hat{\beta}_i(\ell)}{\sum_{i \in \mathcal{I}} \hat{\beta}_i(\ell)}. \quad (3.2.1)$$

With the fractions computed, the algorithm tries to match its current  $N_i$  with the target allocation  $\lfloor \hat{\alpha}_i(\ell)T' \rfloor$  to the greatest possible extent: if  $N_i$  is below the target, run additional simulations to match its target; otherwise, maintain the current  $N_i$  since consumed budget cannot be refunded. All the mean and variance estimates are updated at the end of each iteration. The process continues iteratively until the total budget is depleted. Finally, the design with the highest sample mean is selected as the output.

Observe that two features of OCBA stand out from Algorithm 1. The first one to notice is the allocation fractions specified by (3.2.1), which is a plug-in estimate of

$$\beta_i := \begin{cases} \sigma_i^2/(\mu_b - \mu_i)^2 & \text{if } i \neq b \\ \sigma_b\sqrt{\sum_{i \neq b} \beta_i^2/\sigma_i^2} & \text{o./w.} \end{cases}, \quad \alpha_i := \frac{\beta_i}{\sum_{i \in \mathcal{I}} \beta_i}. \quad (3.2.2)$$

The fractions in (3.2.2) can be derived by asymptotically maximizing a lower bound of the PCS under a normality assumption (see, e.g., [39]). Moreover, [40] showed that for algorithms using a deterministic allocation of  $N_i = \lfloor \alpha_i T \rfloor$ , such fractions approximately maximize the LD rate of PFS in the case of i.i.d. normal samples. The other feature is sequential allocation, which consists of incrementally allocating the budget, repeatedly updating the estimated fractions  $\hat{\alpha}_i$ , and asymptotically matching the true allocation fractions  $\alpha_i$  as  $T \rightarrow \infty$ . Empirical evidence shows that sequential allocation may be the key to its good finite-sample performance, even though a quantitative analysis is not available due to its highly complex dynamics. In this chapter, we attempt to better understand OCBA by studying its asymptotic behavior, and our results will also shed some light on its finite-sample performance.

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**Algorithm 2** OCBA-D

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- 1: **Input:**  $N_0 \geq 2, T \geq KN_0$ .
  - 2: **Initialization:** Sample each design  $N_0$  times and compute  $\bar{X}_i(0)$  and  $S_i^2(0)$ .  $N_i(0) \leftarrow N_0$ .  $\ell \leftarrow 0$ .
  - 3: **while**  $\sum_{i \in \mathcal{I}} N_i(\ell) < T$  **do**
  - 4:     Compute  $\hat{\alpha}_1(\ell), \dots, \hat{\alpha}_K(\ell)$  using (3.2.1).
  - 5:     Run one replication for design  $i^* = \arg \max_{i \in \mathcal{I}} \{\hat{\alpha}_i(\ell)/N_i(\ell)\}$ .
  - 6:      $N_{i^*}(\ell + 1) \leftarrow N_{i^*}(\ell) + 1$ . Compute  $\bar{X}_{i^*}(\ell + 1)$  and  $S_{i^*}^2(\ell + 1)$ .
  - 7:      $\ell \leftarrow \ell + 1$ .
  - 8: **end while**
  - 9: **Output:**  $\hat{b} = \arg \max_{i \in \mathcal{I}} \bar{X}_i(\ell)$ .
- 

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**Algorithm 3** OCBA-R

---

- 1: **Input:**  $N_0 \geq 2, T \geq KN_0$ .
  - 2: **Initialization:** Sample each design  $N_0$  times and compute  $\bar{X}_i(0)$  and  $S_i^2(0)$ .  $N_i(0) \leftarrow N_0$ .  $\ell \leftarrow 0$ .
  - 3: **while**  $\sum_{i \in \mathcal{I}} N_i(\ell) < T$  **do**
  - 4:     Compute  $\hat{\alpha}_1(\ell), \dots, \hat{\alpha}_K(\ell)$  using (3.2.1).
  - 5:     Draw an independent sample  $U(\ell)$  from  $\text{Uniform}(0, 1)$ .
  - 6:     Run one replication for design  $i^* = \min\{k \mid U(\ell) \leq \sum_{i=1}^k \hat{\alpha}_i(\ell), 1 \leq k \leq K\}$ .
  - 7:      $N_{i^*}(\ell + 1) \leftarrow N_{i^*}(\ell) + 1$ . Compute  $\bar{X}_{i^*}(\ell + 1)$  and  $S_{i^*}^2(\ell + 1)$ .
  - 8:      $\ell \leftarrow \ell + 1$ .
  - 9: **end while**
  - 10: **Output:**  $\hat{b} = \arg \max_{i \in \mathcal{I}} \bar{X}_i(\ell)$ .
- 

In addition to OCBA, we also consider variations on OCBA and propose two variants, OCBA-D and OCBA-R, which are presented in Algorithms 2 and 3, respectively. The “D” and “S” stand for “Deterministic” and “Randomized”. Both variants inherit the fractions in (3.2.1) and are designed to be fully sequential, i.e., at each iteration only a single additional run is allocated to some design  $i^*$ . However, their difference lies in the way  $i^*$  is chosen. For OCBA-D,  $i^*$  corresponds to the design with the largest ratio  $\hat{\alpha}_i(\ell)/N_i(\ell)$ , where the ratio is roughly a measure of need for simulations: intuitively, an undersampled design is reflected by a larger ratio relative to the others’. In OCBA-R,  $i^*$  is chosen randomly by using the fractions as a sampling distribution. In other words, conditional on the  $\hat{\alpha}$  vector, the choice of  $i^*$  is independent of everything else. In sum, all three algorithms are governed by the “asymptotically optimal” fractions given by (3.2.2), except that they use

different sequential allocation strategies to approximate such fractions.

We consider OCBA-D and OCBA-R for two reasons. First, fully sequential allocation and randomization are among the most natural forms of generalization to consider, examples including the most-starving version of OCBA ([78]) and the Top-two Sampling Algorithms ([43]). It is therefore important to know if any finding for OCBA also applies to these variants. Second, such variations can often make the algorithm behave more regularly and thus more amenable to analysis.

### 3.2.2 Convergence Analysis

As a main contribution of this chapter, we formally analyze the performance of OCBA, OCBA-D and OCBA-R. Firstly, we show that all three algorithms attain the “asymptotically optimal” allocation fractions given by (3.2.2) as  $T \rightarrow \infty$ . Secondly, we reveal that despite the convergence of fractions, if the initial sample size  $N_0$  is chosen as a constant independent of  $T$ , then these algorithms suffer from a sub-exponential convergence rate.

To put our work in perspective, [40] were among the first to study the asymptotics of fixed budget R&S algorithms. They established that if an algorithm pre-specifies some fractions  $\alpha_i > 0$  and simply sets  $N_i = \lfloor \alpha_i T \rfloor$ , then the PFS converges exponentially fast under weak assumptions on the sample distributions’ tails. In particular, if the samples are i.i.d. normal, then the fractions given by (3.2.2) approximately maximize the LD rate of the PFS. Perhaps under the influence of such insights, there seems to be an implicit conjecture that algorithms which “asymptotically” attain the optimal allocation fractions, such as OCBA, should enjoy a similar LD rate to its static counterpart’s, or at least guarantee exponential convergence. In what follows, we disprove this conjecture by using OCBA and the two proposed variants as counterexamples.

To set the basis for our major discovery, we link Algorithms 1-3 through the convergence of their actual allocation fractions  $N_i(\ell)/\sum_j N_j(\ell)$ . Observe that  $T \rightarrow \infty$  if and only if  $\ell \rightarrow \infty$ , so we characterize such convergence in terms of  $\ell$  for convenience. All the

proofs omitted in the chapter can be found in the electronic companion.

**Proposition 3.2.1.** *Let Assumption 3.1.1 hold and denote “almost surely” by “a.s.”. Then, for OCBA, OCBA-D and OCBA-R, the following holds.*

- (i)  $N_i(\ell) \rightarrow \infty$  a.s. as  $\ell \rightarrow \infty$  for all  $i \in \mathcal{I}$ .
- (ii)  $\hat{\alpha}_i(\ell) \rightarrow \alpha_i$  a.s. as  $\ell \rightarrow \infty$  for all  $i \in \mathcal{I}$ .
- (iii)  $N_i(\ell) / \sum_{j \in \mathcal{I}} N_j(\ell) \rightarrow \alpha_i$  a.s. as  $\ell \rightarrow \infty$  for all  $i \in \mathcal{I}$ .

*Proof of Proposition 3.2.1.* Since (ii) is a direct consequence of (i) due to the consistency of mean and variance estimators, we will show (i) and (iii) for OCBA, OCBA-D, and OCBA-R.

### 1. Proof for OCBA.

- (i) Suppose that all the random variables are defined on a probability space  $(\Omega, \mathcal{F}, \mathbb{P})$ .

By the Strong Law of Large Numbers (SLLN), there exists a measurable set  $\Omega_1 \subseteq \Omega$  such that  $\mathbb{P}(\Omega_1) = 1$  and for all  $\omega \in \Omega_1$  and any design  $i \in \mathcal{I}$ ,

- (1)  $\bar{X}_{i,n} \rightarrow \mu_i$  and  $S_{i,n} \rightarrow \sigma_i$  as  $n \rightarrow \infty$ .
- (2)  $S_{i,n} > 0$  for all  $n \geq 2$ .
- (3)  $\bar{X}_{i,n} \neq \bar{X}_{j,m}$  for all  $j \neq i$  and  $n, m \geq 1$ .

Since the samples follow nondegenerate normal distributions, (2) and (3) both occur with probability 1, and  $\Omega_1$  is guaranteed to exist. Here we mainly need (2) and (3) to avoid some trivial edge cases for OCBA.

Take any sample path  $\omega \in \Omega_1$ . We will show that on  $\omega$ ,  $N_i(\ell) \rightarrow \infty$  as  $\ell \rightarrow \infty$  for all designs. Assume for a contradiction that this does not hold, then there exists a nonempty set  $\tilde{\mathcal{I}} \subseteq \mathcal{I}$  such that  $N_j(\ell) \not\rightarrow \infty$  for all  $j \in \tilde{\mathcal{I}}$ . This means that for all  $j \in \tilde{\mathcal{I}}$ ,  $\bar{X}_j(\ell)$  and  $S_j(\ell)$  will be fixed at some constants for all  $\ell$  large enough. Under this assumption, we claim that the following holds.



**Claim 3.2.1.** *There exists a constant  $\tilde{\alpha} > 0$  such that for all designs  $i \in \mathcal{I}$ ,  $\hat{\alpha}_i(\ell) > \tilde{\alpha}$  for all  $\ell$  large enough.*

*Proof of Claim 3.2.1.* It suffices to show that every  $\hat{\alpha}_i(\ell)$  converges to some positive constant. Note that  $\bar{X}_i(\ell) \rightarrow \mu_i$  and  $S_i(\ell) \rightarrow \sigma_i$  as  $\ell \rightarrow \infty$  for all  $i \in \mathcal{I} \setminus \tilde{\mathcal{I}}$ . Since  $\mu_i \neq \mu_j$  for all  $i \neq j$ , we further know that for all  $\ell$  large enough,  $\hat{b}$  will be fixed and so does the form of  $\hat{\beta}_i$  (note that  $\hat{\beta}_{\hat{b}}$  has a different form than the other  $\hat{\beta}_i$ 's). It then follows from the continuity of  $\hat{\beta}_i$  in  $(\bar{X}_i, S_i)_{i \in \mathcal{I}}$  that  $\hat{\beta}_i(\ell)$  will converge to some constant  $\tilde{\beta}_i > 0$ , and  $\hat{\alpha}_i(\ell) \rightarrow \tilde{\beta}_i / (\sum_{i \in \mathcal{I}} \tilde{\beta}_i) > 0$ .  $\square$

However, when  $T'(\ell)$  gets sufficiently large, we would have

$$\lfloor \hat{\alpha}_j T'(\ell) \rfloor \geq \lfloor \tilde{\alpha} T'(\ell) \rfloor > N_j(\ell)$$

for some design  $j \in \tilde{\mathcal{I}}$ , where step 6 of Algorithm 1 will allocate additional budget to  $j$ , hence a contradiction.

- (iii) Similarly, we will show convergence on  $\Omega_1$ . Let  $\epsilon$  be an arbitrary positive number. From (ii), there exists  $\ell_0$  such that  $\hat{\alpha}_i(\ell) \in [\alpha_i - \epsilon, \alpha_i + \epsilon]$  for all  $\ell \geq \ell_0$ . Furthermore, since  $N_i(\ell) \rightarrow \infty$  for any design  $i$ , we can find  $\ell_i \geq \ell_0$  such that  $N_i(\ell_i + 1) > N_i(\ell_i)$ , i.e.,  $N_i$  jumps at the  $\ell_i$ th iteration. Let  $\bar{\ell} := \max_{i \in \mathcal{I}} \ell_i$  so that every  $N_i$  has jumped at least once since iteration  $\bar{\ell}$ . We claim that for all  $\ell \geq \bar{\ell}$ ,

$$\lfloor (\alpha_i - \epsilon) T'(\ell) \rfloor \leq N_i(\ell) \leq \lfloor (\alpha_i + \epsilon) T'(\ell) \rfloor, \quad \forall i \in \mathcal{I}. \quad (3.2.3)$$

To see why (3.2.3) holds, first notice from step 7 of Algorithm 1 that

$$N_i(\ell) = \max \{N_i(\ell - 1), \lfloor \hat{\alpha}_i(\ell) T'(\ell) \rfloor\} \geq \lfloor \hat{\alpha}_i(\ell) T'(\ell) \rfloor \geq \lfloor (\alpha_i - \epsilon) T'(\ell) \rfloor,$$

so the first inequality in (3.2.3) holds. For the other inequality, there are two cases to consider. If  $N_i(\ell) = \lfloor \hat{\alpha}_i(\ell)T'(\ell) \rfloor$  then (3.2.3) holds apparently. Otherwise,  $N_i(\ell) = \lfloor \hat{\alpha}_i(\ell')T'(\ell') \rfloor$ , where

$$\ell' := \max\{\tilde{\ell} < \ell \mid N_i(\tilde{\ell} + 1) > N_i(\tilde{\ell})\},$$

which is the iteration corresponding to the most recent jump. We know  $\ell_i$  corresponds to a jump, so  $\ell_i \leq \ell' < \ell$ . Since  $\ell_i \geq \ell_0$ , the definition of  $\ell_0$  ensures that  $\hat{\alpha}_i(\ell') \leq \alpha_i + \epsilon$ . Thus,

$$N_i(\ell) = \lfloor \hat{\alpha}_i(\ell')T'(\ell') \rfloor \leq \lfloor (\alpha_i + \epsilon)T'(\ell) \rfloor,$$

so (3.2.3) always holds. This would imply that

$$\frac{\alpha_i - \epsilon}{1 + K\epsilon} \leq \liminf_{\ell \rightarrow \infty} \frac{N_i(\ell)}{\sum_{j \in \mathcal{I}} N_j(\ell)} \leq \limsup_{\ell \rightarrow \infty} \frac{N_i(\ell)}{\sum_{j \in \mathcal{I}} N_j(\ell)} \leq \frac{\alpha_i + \epsilon}{1 - K\epsilon}$$

for all  $\epsilon$  sufficiently small. Send  $\epsilon \rightarrow 0$  and the conclusion follows.

## 2. Proof for OCBA-D.

- (i) Using the  $\Omega_1$  constructed previously, this can be shown by following a similar argument as in OCBA's proof (proof by contradiction).
- (iii) Pick design 1 as reference design. It suffices to show that on  $\Omega_1$ ,  $N_i(\ell)/N_1(\ell) \rightarrow \alpha_i/\alpha_1$  as  $\ell \rightarrow \infty$  for all  $i \neq 1$ . To begin with, for any  $\epsilon > 0$ , there exists  $\ell'$  such that for all  $\ell \geq \ell'$ ,  $\hat{\alpha}_i(\ell) \in [\alpha_i - \epsilon, \alpha_i + \epsilon]$ ,  $\forall i \in \mathcal{I}$ . Furthermore, since  $N_i(\ell)$  is nondecreasing in  $\ell$  and  $N_i(\ell) \rightarrow \infty$  as  $\ell \rightarrow \infty$ , we can find  $\ell'' \geq \ell'$  such that all the designs satisfy  $N_i(\ell) \geq N_i(\ell') + 2$  for all  $\ell \geq \ell''$ , i.e., all the  $N_i$ 's have jumped at least twice since the  $\ell'$ th iteration. Then, we claim that for any design

$i \neq 1$ ,

$$\frac{\alpha_i + \epsilon}{N_i(\ell) - 1} \geq \frac{\alpha_1 - \epsilon}{N_1(\ell)}, \quad \forall \ell \geq \ell''. \quad (3.2.4)$$

Assume for a contradiction that (3.2.4) does not hold. Let

$$\ell_i := \max\{\tilde{\ell} \mid N_i(\tilde{\ell}) = N_i(\ell) - 1\},$$

namely, the iteration when design  $i$  is chosen to be simulated and  $N_i$  is about to jump from  $N_i(\ell) - 1$  to  $N_i(\ell)$ . It then follows from the definition of  $\ell''$  that  $\ell' \leq \ell_i \leq \ell$ , and from step 5 of Algorithm 2 we have

$$\frac{\hat{\alpha}_i(\ell_i)}{N_i(\ell_i)} \geq \frac{\hat{\alpha}_j(\ell_i)}{N_j(\ell_i)}, \quad j \neq i. \quad (3.2.5)$$

However, if (3.2.4) does not hold, then we will have

$$\frac{\hat{\alpha}_i(\ell_i)}{N_i(\ell_i)} \leq \frac{\alpha_i + \epsilon}{N_i(\ell) - 1} < \frac{\alpha_1 - \epsilon}{N_1(\ell)} \leq \frac{\hat{\alpha}_1(\ell_i)}{N_1(\ell_i)},$$

hence a contradiction to (3.2.5). Thus, (3.2.4) provides an upper bound on  $N_i(\ell)$ .

$$N_i(\ell) \leq \left( \frac{\alpha_i + \epsilon}{\alpha_1 - \epsilon} \right) N_i(\ell) + 1. \quad (3.2.6)$$

By symmetry (using design  $i$  as a reference design), we also have

$$\frac{\alpha_1 + \epsilon}{N_1(\ell) - 1} \geq \frac{\alpha_i - \epsilon}{N_i(\ell)}, \quad \forall \ell \geq \ell'',$$

which gives the following lower bound on  $N_i(\ell)$ .

$$N_i(\ell) \geq \left( \frac{\alpha_i - \epsilon}{\alpha_1 + \epsilon} \right) (N_1(\ell) - 1). \quad (3.2.7)$$

Combining (3.2.6) and (3.2.7) and we have

$$\frac{\alpha_i - \epsilon}{\alpha_1 + \epsilon} \leq \liminf_{\ell \rightarrow \infty} \frac{N_i(\ell)}{N_1(\ell)} \leq \limsup_{\ell \rightarrow \infty} \frac{N_i(\ell)}{N_1(\ell)} \leq \frac{\alpha_i + \epsilon}{\alpha_1 - \epsilon}.$$

Take  $\epsilon \rightarrow 0$  and we conclude that  $N_i(\ell)/N_1(\ell) \rightarrow \alpha_i/\alpha_1$  as  $\ell \rightarrow \infty$ .

### 3. Proof for OCBA-R.

(i) Let  $\mathbb{1}_{\{\cdot\}}$  denote an indicator function. Define an event

$$\Omega_2 := \bigcap_{n \geq 1} \bigcap_{0 \leq m \leq n-1} \left\{ \omega \in \Omega \left| \lim_{\ell \rightarrow \infty} \frac{1}{\ell} \sum_{\ell} \mathbb{1}_{\{U(\ell) \in [\frac{m}{n}, \frac{m+1}{n}]\}} = \frac{1}{n} \right. \right\},$$

which has probability 1 due to SLLN. We will show that  $N_i(\ell) \rightarrow \infty$  as  $\ell \rightarrow \infty$  on  $\Omega_3 := \Omega_1 \cap \Omega_2$ . Assume for a contradiction that this is not true. By an argument similar to OCBA's proof,  $\hat{\alpha}_i(\ell) \rightarrow \tilde{\alpha}_i$  as  $\ell \rightarrow \infty$  for some  $\tilde{\alpha}_i > 0$ . Then, any design  $i$  will be simulated if and only if  $U(\ell)$  falls into some nonempty interval  $I_i(\ell)$ . We can find  $n_i, m_i, k_i \geq 0$  such that  $[\frac{m_i}{n_i}, \frac{m_i+k_i}{n_i}] \subseteq I_i(\ell)$  for all  $\ell$  large enough, and the definition of  $\Omega_2$  ensures that

$$\liminf_{\ell \rightarrow \infty} \frac{1}{\ell} \sum_{\ell} \mathbb{1}_{\{U(\ell) \in I_i\}} \geq \lim_{\ell \rightarrow \infty} \frac{1}{\ell} \sum_{\ell} \mathbb{1}_{\{U(\ell) \in [\frac{m_i}{n_i}, \frac{m_i+k_i}{n_i}]\}} = \frac{k_i}{n_i},$$

so all the designs will be simulated infinitely often, which is a contradiction.

(iii) It follows from (i) that for any arbitrary  $\epsilon > 0$ , there exists  $\ell'$  such that for all designs,  $\hat{\alpha}_i(\ell) \in [\alpha_i - \epsilon, \alpha_i + \epsilon]$  for all  $\ell \geq \ell'$ . Meanwhile, at each iteration  $\ell$ , design  $i$  is simulated if and only if  $U(\ell) \in I_i(\ell) := [\sum_{j=0}^{i-1} \hat{\alpha}_j(\ell), \sum_{j=0}^i \hat{\alpha}_j(\ell)]$ , where we let  $\hat{\alpha}_0(\ell) := 0, \forall \ell$ . Also define  $I_i^{-\epsilon} := [\sum_{j=0}^{i-1} \alpha_j + (i-1)\epsilon, \sum_{j=0}^i \alpha_j - i\epsilon]$  and  $I_i^{\epsilon} := [\sum_{j=0}^{i-1} \alpha_j - (i-1)\epsilon, \sum_{j=0}^i \alpha_j + i\epsilon]$ . We may assume that  $\epsilon$  is sufficiently small so that  $I_i^{-\epsilon}$  and  $I_i^{\epsilon}$  are both well-defined. It follows that  $I_i^{-\epsilon} \subseteq I_i(\ell) \subseteq I_i^{\epsilon}$  for all  $\ell \geq \ell'$ . Furthermore, there exists intervals  $I'_i$  and

$I_i''$  (independent of  $\ell$ ) with rational endpoints such that  $I_i' \subseteq I_i^{-\epsilon} \subseteq I_i^\epsilon \subseteq I_i''$ ,  $|I_i^{-\epsilon} \setminus I_i'| \leq \epsilon$  and  $|I_i'' \setminus I_i^\epsilon| \leq \epsilon$ . Combining all these and by the definition of  $\Omega_2$ ,

$$\begin{aligned} \alpha_i - 2i\epsilon &= \lim_{\ell \rightarrow \infty} \frac{1}{\ell} \sum_{\ell} \mathbb{1}_{\{U(\ell) \in I_i'\}} \leq \liminf_{\ell \rightarrow \infty} \frac{1}{\ell} \sum_{\ell} \mathbb{1}_{\{U(\ell) \in I_i(\ell)\}} \\ &\leq \limsup_{\ell \rightarrow \infty} \frac{1}{\ell} \sum_{\ell} \mathbb{1}_{\{U(\ell) \in I_i(\ell)\}} \leq \lim_{\ell \rightarrow \infty} \frac{1}{\ell} \sum_{\ell} \mathbb{1}_{\{U(\ell) \in I_i''\}} = \alpha_i + 2i\epsilon. \end{aligned}$$

Send  $\epsilon \rightarrow 0$  and we have  $\frac{1}{\ell} \sum_{\ell} \mathbb{1}_{\{U(\ell) \in I_i(\ell)\}} \rightarrow \alpha_i$  as  $\ell \rightarrow \infty$ . The conclusion follows immediately from the fact that  $N_i(\ell) = N_0 + \sum_{\ell \geq 0} \mathbb{1}_{\{U(\ell) \in I_i(\ell)\}}$ .

□

Proposition 3.2.1 is not surprising since all three algorithms are designed to approximate and match the true fractions  $\alpha_i$  in (3.2.2). It holds regardless of the value of  $N_0$  (as long as  $N_0 \geq 2$ ), because the algorithms are capable of correcting the estimation error from the initialization phase. For this reason, a small  $N_0$  is often employed to leave room for better allocation flexibility in succeeding iterations. For example, a common suggestion for  $N_0$  is between 5 and 20 (see, e.g., [79, 80]). Nevertheless, the following theorem suggests that a constant  $N_0$  independent of  $T$  can cause the PFS to converge rather slowly.

**Theorem 3.2.1.** *Let Assumption 3.1.1 hold. If  $N_0$  is chosen as a constant independent of  $T$ , then for OCBA and OCBA-D,*

$$PFS(T) \geq CT^{-(K-1)(N_0-1)}, \quad \forall T \geq KN_0, \quad (3.2.8)$$

*for some constant  $C > 0$  independent of  $T$ . Also, for OCBA-R,*

$$-\lim_{T \rightarrow \infty} \frac{1}{T} \log PFS(T) = 0. \quad (3.2.9)$$

Theorem 3.2.1 appears somewhat surprising, as it states that a constant initial sample size leads to at most a polynomial convergence rate for OCBA and OCBA-D, and a

sub-exponential convergence rate for OCBA-R. At a high level, it implies that the initial estimation error, though vanishing as  $T \rightarrow \infty$ , does not decrease at a sufficiently fast rate. It also implies that the convergence of allocation fractions alone does not say much about how fast the PFS converges. Before showing Theorem 3.2.1, we present a few technical lemmas and describe the main idea behind the proof.

**Lemma 3.2.1.** *Let  $S_n$  be the sample standard deviation of  $n$  i.i.d. normal samples with variance  $\sigma^2$ . Then, for any  $0 < x < \sigma$ ,*

$$\mathbb{P}(S_n \leq \sigma - x) \leq \exp \left\{ -\frac{(n-1)}{4} \left[ 1 - \left( \frac{\sigma - x}{\sigma} \right)^2 \right]^2 \right\}, \quad (3.2.10)$$

$$\mathbb{P}(S_n \geq \sigma + x) \leq \exp \left( -\frac{(n-1)x^2}{4\sigma^2} \right), \quad \forall x > 0. \quad (3.2.11)$$

*Proof of Lemma 3.2.1.* According to Lemma 1 in [81], if  $X \sim \chi^2(n)$ , then

$$\mathbb{P}(X - n \leq -2\sqrt{nx}) \leq e^{-x}, \quad \forall x > 0,$$

$$\mathbb{P}(\chi^2(n) - n \geq 2\sqrt{nx} + 2x) \leq e^{-x}, \quad \forall x > 0.$$

Since  $(n-1)S_n/\sigma^2 \sim \chi^2(n-1)$ , (3.2.10) and (3.2.11) can be derived by a change of variable.  $\square$

**Lemma 3.2.2.** *Let  $S_n^2$  be the sample variance of  $n$  i.i.d.  $\mathcal{N}(\mu, \sigma^2)$  random variables. Then,  $\forall c > 0, \exists \bar{\epsilon} \in (0, \sigma)$  such that*

$$\sum_{n \geq 2} \mathbb{P}\{S_n \leq \sigma - \bar{\epsilon}\} \leq c. \quad (3.2.12)$$

*Proof of Lemma 3.2.2.* Fix  $\epsilon$  as some arbitrary number in  $(0, \sigma)$ . From Lemma 3.2.1 we know that  $\mathbb{P}\{S_n \leq \sigma - \epsilon\} \leq C_\epsilon e^{-\gamma_\epsilon n}, \forall \epsilon \in (0, \sigma)$ , where  $\gamma_\epsilon := \frac{1}{4} \left[ 1 - \left( \frac{\sigma - \epsilon}{\sigma} \right)^2 \right]^2$  and

$C_\epsilon := e^{\gamma_\epsilon}$ . Thus,  $\exists L \geq 1$  such that

$$\sum_{n \geq L} \mathbb{P}\{S_n \leq \sigma - \epsilon\} \leq \frac{C_\epsilon e^{-\gamma_\epsilon L}}{1 - e^{-\gamma_\epsilon}} \leq \frac{c}{2}.$$

If  $L = 2$ , then set  $\bar{\epsilon} = \epsilon$  and (3.2.12) holds. Otherwise, since  $\mathbb{P}\{S_n \leq \sigma - \epsilon\} \downarrow 0$  as  $\epsilon \uparrow \sigma$ ,  $\exists \epsilon' \in (0, \sigma)$  such that  $\sum_{n=m}^{L-1} \mathbb{P}\{S_n \leq \sigma - \epsilon'\} \leq c/2$ . Take  $\bar{\epsilon} := \max\{\epsilon, \epsilon'\}$  and we have

$$\begin{aligned} \sum_{n \geq m} \mathbb{P}\{S_n \leq \sigma - \bar{\epsilon}\} &\leq \sum_{n=m}^{L-1} \mathbb{P}\{S_n \leq \sigma - \bar{\epsilon}\} + \sum_{n \geq L} \mathbb{P}\{S_n \leq \sigma - \bar{\epsilon}\} \\ &\leq \frac{c}{2} + \sum_{n \geq L} \mathbb{P}\{S_n \leq \sigma - \epsilon\} \leq c, \end{aligned}$$

so that (3.2.12) also holds. □

**Lemma 3.2.3.** *Let  $S_n^2$  be the sample variance of  $n$  i.i.d.  $\mathcal{N}(\mu, \sigma^2)$  random variables. Then,  $\forall a \in (0, b)$ , where  $b > 0$  is a constant,  $\exists \mathcal{K}_b > 0$  such that*

$$\mathbb{P}\{S_n \leq a\} \geq (\mathcal{K}_b a)^{n-1}.$$

*Proof of Lemma 3.2.3.* Note that  $(n-1)S_n^2/\sigma^2 \sim \chi^2(n-1)$ . Let  $Z_1, Z_2, \dots$  be i.i.d.  $\mathcal{N}(0, 1)$  random variables, and we have

$$\begin{aligned} \mathbb{P}\{S_n \leq a\} &= \mathbb{P}\left\{\frac{(n-1)S_n^2}{\sigma^2} \leq \frac{(n-1)a^2}{\sigma^2}\right\} = \mathbb{P}\left\{\sum_{i=1}^{n-1} |Z_i|^2 \leq \frac{(n-1)a^2}{\sigma^2}\right\} \\ &\geq \mathbb{P}\left\{\bigcap_{i=1}^{n-1} \left\{|Z_i| \leq \frac{a}{\sigma}\right\}\right\} = \left[\mathbb{P}\left\{|Z_1| \leq \frac{a}{\sigma}\right\}\right]^{n-1}, \end{aligned}$$

where we observe that

$$\mathbb{P}\left\{|Z_1| \leq \frac{a}{\sigma}\right\} \geq \frac{2a}{\sigma} \frac{1}{\sqrt{2\pi}} e^{-\frac{a^2}{2\sigma^2}} \geq \left(\frac{2e^{-\frac{b^2}{2\sigma^2}}}{\sigma\sqrt{2\pi}}\right) a := \mathcal{K}_b a,$$

by inspecting the shape of normal distribution's density, □

Lemma 3.2.1 provides some basic tail bounds for the standard deviation estimator  $S_n$ , which can be used to prove Lemma 3.2.2. Lemma 3.2.3 is the leading cause behind the polynomial convergence rate for OCBA and OCBA-D, as it points out that the left tail of  $S_n$  converges to 0 only at a polynomial rate. To illustrate the main idea behind the proof of Theorem 3.2.1, consider an adversarial scenario for OCBA where

1. After the initialization phase,  $\hat{b}$  is some suboptimal design, e.g., design 2.
2. The algorithm allocates all the remaining budget to design 2.
3. The sample mean of design 2 beats all other designs' over all iterations.

In the scenario described above, we say that the algorithm “freezes” all the designs other than design 2, which only happens if the initial estimates for the “frozen” designs are highly inaccurate. For instance, we may consider a case where for all  $i \neq 2$ ,  $S_i(0)$  takes very small value and thus  $\hat{\alpha}_i(\ell)$  is also tiny. This would trick the algorithm into greedily sampling design 2, while all the other designs' mean and variance estimates get no further update and thus stay inaccurate. To avoid technicalities, we further require design 2 to be the observed best design throughout the allocation process, so that  $\hat{\alpha}_2(\ell)$  takes the same functional form for any iteration  $\ell$  (recall from (3.2.1) that  $\hat{\alpha}_{\hat{b}}(\ell)$  has a different form than  $\hat{\alpha}_i(\ell), i \neq \hat{b}$ ). The rest is to bound the probability of such an event from below, and show that it is not exponentially rare.

*Proof of Theorem 3.2.1.*

1. **Proof for OCBA.** Assume without loss of generality that  $\mu_1 > \mu_2 > \dots > \mu_K$ . For each design  $i$ , we will construct events  $E_i(T)$  such that on  $\mathcal{E}(T) := \bigcap_{i=1}^K E_i(T)$ , a false selection always occurs. Without ambiguity, we will simply drop  $T$  and write  $\mathcal{E}$  and  $E_i$  instead. To begin with, by Lemma 3.2.2 we can choose  $\bar{\epsilon} \in (0, \sigma_2)$  such that  $\sum_{n \geq N_0} \mathbb{P}\{S_{2,n} \leq \sigma_2 - \bar{\epsilon}\} \leq 1/4$ . By a similar argument, there exists  $\bar{\eta} > 0$  such that



$\sum_{n \geq N_0} \mathbb{P}\{\bar{X}_{2,n} \leq \mu_2 - \bar{\eta}\} \leq 1/4$ . Let

$$E_2 := \{\bar{X}_{2,n} \geq \mu_2 - \bar{\eta}, \forall n \geq N_0\} \cap \{S_{2,n} \geq \sigma_2 - \bar{\epsilon}, \forall n \geq N_0\}.$$

Then,  $\mathbb{P}(E_2) \geq 1 - \frac{1}{4} - \frac{1}{4} = \frac{1}{2}$  by a union bound. For  $i \neq 2$ , we let

$$E_i := \{\bar{X}_{i,N_0} \leq \mu_2 - \bar{\eta} - 1\} \cap \{S_{i,N_0} \leq N_0(\sigma_2 - \bar{\epsilon})/T\}.$$

We now show that  $\bigcap_{i=1}^K E_i \subseteq \text{FS}$  by induction, where “FS” stands for the false selection event. Fix a sample path on  $E_i$ . Note that  $\hat{b} = 2$  after the initialization phase. Assume that  $\hat{b} = 2$  at the end of the  $(\ell - 1)$ th iteration, then at the  $\ell$ th iteration, for any  $i \neq 2$ ,

$$\begin{aligned} \hat{\alpha}_i(\ell) &= \frac{S_i^2(\ell)/\hat{\delta}_{2,i}^2(\ell)}{\sum_{j \neq 2} \frac{S_j^2(\ell)}{\hat{\delta}_{2,j}^2(\ell)} + S_2(\ell) \sqrt{\sum_{j \neq 2} \frac{S_j^2(\ell)}{\hat{\delta}_{2,j}^4(\ell)}}} \leq \frac{S_i^2(\ell)/\hat{\delta}_{2,i}^2(\ell)}{S_2(\ell) \sqrt{\frac{S_i^2(\ell)}{\hat{\delta}_{2,i}^4(\ell)}}} \\ &= \frac{S_i(\ell)}{S_2(\ell)} \leq \frac{N_0(\sigma_2 - \bar{\epsilon})}{S_2(\ell)T}, \end{aligned}$$

where  $\hat{\delta}_{i,j}(\ell) := \bar{X}_i(\ell) - \bar{X}_j(\ell)$ . From  $E_2$  we have  $S_2(\ell) \geq \sigma_2 - \bar{\epsilon}$ , thus  $\hat{\alpha}_i(\ell)T'(\ell) \leq \hat{\alpha}_i(\ell)T \leq N_0$  for all  $i \neq 2$  and only design 2 will get additional sample at step 7 of Algorithm 1. Since  $\bar{X}_2(\ell) \geq \mu - \bar{\eta} > \mu_2 - \bar{\eta} - 1 \geq \bar{X}_{i,N_0} = \bar{X}_i(\ell)$  for all  $i \neq 2$ , design 2 will still be  $\hat{b}$  at the end of the  $\ell$ th iteration. Continue this process and a false selection is certain when the algorithm terminates. Finally, the probability of  $\mathcal{E}$  can be bounded from below as follows.

$$\begin{aligned} \mathbb{P}(\mathcal{E}) &= \mathbb{P}\left(\bigcap_{i=1}^K E_i\right) = \prod_{i=1}^K \mathbb{P}(E_i) \geq \frac{1}{2} \prod_{i \neq 2} \mathbb{P}(E_i) \\ &= \frac{1}{2} \prod_{i \neq 2} \left[ \underbrace{\mathbb{P}\{\bar{X}_{i,N_0} \leq \mu_2 - \bar{\eta} - 1\}}_{(\dagger)} \underbrace{\mathbb{P}\left\{S_{i,N_0} \leq \frac{N_0(\sigma_2 - \bar{\epsilon})}{T}\right\}}_{(\dagger\dagger)} \right], \end{aligned}$$

where the last equality follows from the independence of  $\bar{X}_{i,N_0}$  and  $S_{i,N_0}$ . Furthermore,  $(\dagger) \geq p_i$  for some constant  $p_i > 0$  (independent of  $T$ ), and  $(\dagger\dagger) \geq [\mathcal{K}_i(\sigma_2 - \bar{\epsilon})/T]^{N_0-1}$  by Lemma 3.2.3, where  $\mathcal{K}_i > 0$  are constants independent of  $T$ . Gather all the terms and the conclusion follows.

2. **Proof for OCBA-D.** For OCBA-D, we use the same construction of events  $E_i$  as in OCBA's proof. It suffices to show inductively that  $\hat{b} = i^* = 2$  for all iterations  $\ell$ . We know that this is true at  $\ell = 0$ . Assume that it holds for the  $(\ell - 1)$ th iteration. Then, at the  $\ell$ th iteration, we have for all  $i \neq 2$ ,

$$\begin{aligned} \frac{\hat{\alpha}_i(\ell)}{\hat{\alpha}_2(\ell)} &= \frac{S_i^2(\ell)/\hat{\delta}_{2,i}^2(\ell)}{S_2(\ell)\sqrt{\sum_{j \neq 2} \frac{S_j^2(\ell)}{\hat{\delta}_{2,j}^4(\ell)}}} \leq \frac{S_i^2(\ell)/\hat{\delta}_{2,i}^2(\ell)}{S_2(\ell)\sqrt{\frac{S_i^2(\ell)}{\hat{\delta}_{2,i}^4(\ell)}}} \\ &= \frac{S_i(\ell)}{S_2(\ell)} \leq \frac{N_0(\sigma_2 - \bar{\epsilon})}{S_2(\ell)T} \leq \frac{N_0}{T}, \end{aligned} \quad (3.2.13)$$

which implies that

$$\frac{\hat{\alpha}_i(\ell)}{N_i(\ell)} = \frac{\hat{\alpha}_i(\ell)}{N_0} \leq \frac{\hat{\alpha}_2(\ell)}{T} < \frac{\hat{\alpha}_2(\ell)}{N_2(\ell)}, \quad \forall i \neq 2.$$

Thus,  $i^* = 2$  and  $\hat{b} = 2$  at the  $\ell$ th iteration, and the process will eventually lead to a false selection. The rest follows from the same argument in OCBA's proof.

3. **Proof for OCBA-R.** Next, we prove (3.2.9) for OCBA-R. Fix an arbitrary  $\epsilon \in (0, 1)$ . The event  $E_2$  uses the same construction as in OCBA's proof, i.e.,

$$E_2 := \left\{ \bar{X}_{2,n} \geq \mu_2 - \bar{\eta}, \forall n \geq N_0 \right\} \cap \left\{ S_{2,n} \geq \sigma_2 - \bar{\epsilon}, \forall n \geq N_0 \right\},$$

where  $\bar{\eta} > 0$  and  $\bar{\epsilon} \in (0, \sigma_2)$  are chosen such that  $\mathbb{P}(E_2) \geq 1/2$ . For  $i \neq 2$ , we let

$$E_i := \left\{ \bar{X}_{i,N_0} \leq \mu_2 - \eta - 1 \right\} \cap \left\{ S_{i,N_0} \leq \epsilon(\sigma_2 - \bar{\epsilon})/(K - 1) \right\}.$$

Let  $\mathcal{E} := \bigcap_{i=1}^K E_i$  and  $L := T - KN_0 - 1$ . Note that if  $\mathcal{E}$  occurs and the algorithm picks  $i^* = 2$  at all iterations, then a false selection always occurs. This provides a lower bound for the PFS,

$$\begin{aligned}
\text{PFS}(T) &\geq \mathbb{P} \{ \{i^* = 2, \forall \ell = 0, \dots, L\} \cap \mathcal{E} \} \\
&= \mathbb{P} \left\{ \left\{ i^* = \hat{b} = 2, \forall \ell = 0, \dots, L \right\} \cap \mathcal{E} \right\} \\
&= \mathbb{E} \left[ \prod_{\ell=0}^L \hat{\alpha}_2(\ell) \mathbb{1}_{\mathcal{E}} \right], \tag{3.2.14}
\end{aligned}$$

where the last inequality follow from the design of Algorithm 3, and

$$\hat{\alpha}_2(\ell) = \frac{S_2(\ell) \sqrt{\sum_{j \neq 2} \frac{S_j^2(\ell)}{\hat{\delta}_{2,j}^4(\ell)}}}{\sum_{j \neq 2} \frac{S_j^2(\ell)}{\hat{\delta}_{2,j}^2(\ell)} + S_2(\ell) \sqrt{\sum_{j \neq 2} \frac{S_j^2(\ell)}{\hat{\delta}_{2,j}^4(\ell)}}}, \quad \forall \ell = 0, \dots, L,$$

since  $\hat{b} = 2$  for all  $\ell = 0, \dots, L$ . Furthermore, on event  $\mathcal{E}$  we have

$$\hat{\alpha}_i(\ell) \leq \frac{\hat{\alpha}_i(\ell)}{\hat{\alpha}_2(\ell)} \leq \frac{S_i(\ell)}{S_2(\ell)} = \frac{S_{i,N_0}}{S_2(\ell)} \leq \frac{\epsilon(\sigma_2 - \bar{\epsilon})}{(K-1)(\sigma_2 - \bar{\epsilon})} \leq \frac{\epsilon}{K-1},$$

where the second inequality follows from (3.2.13), the equality follows from  $i^* = 2$  for all  $\ell = 0, \dots, L$ , and the third inequality is a consequence of  $E_2$  and  $E_i$ . Thus,  $\hat{\alpha}_2(\ell) = 1 - \sum_{i \neq 2} \hat{\alpha}_i(\ell) \geq 1 - \epsilon$  for  $\ell = 0, \dots, L$ , and plugging it into (3.2.14) gives

$$\text{PFS}(T) \geq \mathbb{P}(\mathcal{E})(1 - \epsilon)^{T - KN_0},$$

where  $\mathbb{P}(\mathcal{E}) = \prod_{i=1}^K \mathbb{P}(E_i) > 0$  is a constant independent of  $T$ . Therefore,

$$-\lim_{T \rightarrow \infty} \frac{1}{T} \log \text{PFS}(T) \leq -\log(1 - \epsilon).$$

Take  $\epsilon \downarrow 0$  and (3.2.9) follows.

□

The key to proving Theorem 3.2.1 is to exploit the asymmetry of the standard deviation estimator's distribution. Specifically, when constructing events  $E_i(T)$ , we require  $S_{i,N_0}$  to decrease in order  $1/T$  as  $T \rightarrow \infty$  for all  $i \neq 2$ . Then, Lemma 3.2.3 can be used to show a polynomial lower bound for  $\mathbb{P}(E_i)$ . Another way to construct a “freezing” event is by increasing  $S_2(\ell)$  in order  $T$ , but this merely produces an exponential lower bound according to (3.2.11) in Lemma 3.2.1. In other words, only exploiting the left tail of  $S_{i,N_0}$  would produce a tighter lower bound for the PFS.

Theorem 3.2.1 can be counterintuitive at first glance. Recall from [40] that for normal samples, any fixed fractions  $\alpha_i > 0$  would guarantee an exponential convergence rate. This particularly includes equal allocation, i.e.,  $N_i = \lfloor T/K \rfloor$  for all designs  $i$ . In this regard, Theorem 3.2.1 seems to suggest that equal allocation is better than more sophisticated sequential allocation procedures, which contradicts numerous empirical studies in which OCBA exhibits significant advantage over equal allocation. To resolve the “conflict”, note that the LD rate is only defined in an asymptotic sense, meaning that when  $T$  gets large enough, equal allocation will eventually achieve a lower PFS than all three OCBA-type algorithms we consider. However, the crossing point of  $T$  may be so large that the PFS is already very close to 0, which also explains why such a crossing point is not always observed in numerical results.

### 3.2.3 A Modification for Improvement

We propose a simple modification to the three OCBA-type algorithms, which is to make  $N_0$  grow linearly in  $T$ . This can be done by choosing a constant  $\alpha_0 \in (0, 1/K)$  and setting  $N_0 = \lfloor \alpha_0 T \rfloor$ . Intuitively, the PFS should converge at least as fast as equally allocating  $\lfloor \alpha_0 T \rfloor$  to all designs, where an exponential convergence is guaranteed. More formally, we have the following finite-sample bound on the PFS.

**Theorem 3.2.2.** *Let Assumption 3.1.1 hold and suppose that  $\mu_1 > \mu_2 > \dots > \mu_K$ . If  $N_0 = \lfloor \alpha_0 T \rfloor$  for some  $\alpha_0 \in (0, 1)$ , then for OCBA, OCBA-D and OCBA-R, there exists some positive constants  $C_1, \dots, C_K$  (independent of  $T$ ) such that*

$$PFS(T) \leq C_1 \exp\left(-\frac{\delta^2 \alpha_0 T}{8\sigma_1^2 K}\right) + \sum_{i=2}^K C_i \exp\left(-\frac{\bar{\delta}_i^2 \alpha_0 T}{2\sigma_i^2 K}\right), \quad \forall T \geq KN_0, \quad (3.2.15)$$

where  $\delta := \mu_1 - \mu_2$  and  $\bar{\delta}_i = \mu_2 - \mu_i + \frac{\delta}{2}$  for  $i = 2, \dots, K$ .

*Proof of Theorem 3.2.2.* Note that since  $N_0 \leq N_i \leq T$  for all designs  $i$ , if the event

$$\mathcal{E} := \bigcap_{r=N_0}^T \left\{ \left\{ \bar{X}_{1,r} \geq \mu_1 - \frac{\delta}{2} \right\} \cap \left\{ \bigcap_{i \neq 1} \{ \bar{X}_{i,r} \leq \mu_i + \bar{\delta}_i \} \right\} \right\}$$

occurs, then we have a correct selection regardless of the exact values of  $N_i$ 's. Apply a Gaussian tail bound for  $\bar{X}$  and we have

$$\begin{aligned} PFS(T) &\leq \mathbb{P}(\mathcal{E}^c) \leq \sum_{r=N_0}^T \left[ \mathbb{P}\left(\bar{X}_{1,r} < \mu_1 - \frac{\delta}{2}\right) + \sum_{i=2}^K \mathbb{P}\left(\bar{X}_{i,r} > \mu_i + \bar{\delta}_i\right) \right] \\ &\leq \sum_{r=N_0}^{\infty} \mathbb{P}\left(\bar{X}_{1,r} < \mu_1 - \frac{\delta}{2}\right) + \sum_{i=2}^K \sum_{r=N_0}^{\infty} \mathbb{P}\left(\bar{X}_{i,r} > \mu_i + \bar{\delta}_i\right) \\ &\leq \sum_{r=N_0}^{\infty} \exp\left(-\frac{\delta^2 r}{8\sigma_1^2}\right) + \sum_{i=2}^K \sum_{r=N_0}^{\infty} \exp\left(-\frac{\bar{\delta}_i^2 r}{2\sigma_i^2}\right). \end{aligned}$$

Evaluate the geometric sums and (3.2.15) follows.  $\square$

The bound (3.2.15) fills the long-standing void of a finite-sample PFS upper bound for OCBA-type algorithms. It also applies to a broad class of algorithms that involve a warm-up phase of acquiring initial estimates. An idea similar to using a linearly increasing  $N_0$  is to enforce hard thresholds for the actual fractions such that, e.g.,  $N_i(\ell) / \sum_j N_j(\ell) > \epsilon_i$  for some  $\epsilon_i > 0$ . Both methods will force  $N_i(\ell)$  to grow at least linearly fast in  $T$ , but we work with the former mainly for conveniently obtaining a PFS bound. The choice of  $\alpha_0$  inevitably involves a tradeoff between lower initial estimation error and higher flexibility

in subsequent allocation. In Section 3.4, we will use numerical results to demonstrate that an appropriately chosen  $\alpha_0$  can lead to a significant improvement in the finite-sample PCS.

One drawback of the finite-sample bound in (3.2.15) is that it is too general and thus can be quite loose. While a tighter upper bound should reflect the pros and cons of different sequential allocation strategies, deriving such a bound is known to be very challenging even for nicely structured fully sequential algorithms. In the upcoming section, we turn our attention to algorithms which follow simple designs yet capture some key features of advanced algorithms. The idea is to examine the individual impact of a feature through LD rate analysis, and keep the intuition uncluttered from other common features in a sophisticated algorithm.

### 3.3 Characterizing the LD Rate for Simplified Algorithms

In this section, we focus on algorithms with an exponential convergence rate, for which the LD rate is one of the most precise quantitative measures of asymptotic behavior. Nevertheless, LD rate analysis remains difficult for sophisticated sequential allocation algorithms. In this section, we *exactly characterize* the LD rate for some simplified algorithms, and compare their LD rates with that achieved by the optimal static allocation derived in [40]. Each algorithm to be considered has a simple structure yet represents certain important feature of more advanced algorithms. Our analysis will focus on a two-design case for better tractability, but the proof techniques and insights can provide a basis for more general convergence analysis.

#### 3.3.1 Algorithms Overview

We consider a case of  $K = 2$  and study three algorithms, which are presented in Algorithms 4-6. Algorithm 4 is the deterministic algorithm studied in [40], which statically allocates the budget according to pre-specified fractions  $p$  and  $1 - p$ , hence the name “deterministic static (DS)”.

A slight modification of DS leads to the randomized static (RS) algorithm in Algorithm 5, which uses the static fractions as a sampling probability distribution at every iteration, and thus can be roughly regarded as a simplified version of OCBA-R or the Top-two Sampling Algorithms in [43]. To the best of our knowledge, the (frequentist) convergence rate of such a randomized algorithm has not been studied in the literature.

Finally, Algorithm 6 is a two-phase algorithm which uses phase I to estimate the optimal DS fractions (see Section 3.3.2 for more details), and then implements the estimated fractions in phase II. The two-phase algorithm is a vanilla version of our modified OCBA-type algorithms, as it enforces a linearly growing  $N_0$ , but does not update the fraction estimates in all subsequent iterations. Also, notice that we do not reuse the initial  $2N_0$  samples in phase II, so  $N_1$  and  $N_2$  are not bounded from below by a linear function of  $T$  and Theorem 3.2.2 does not apply. However, we will show that it still has an exponential convergence rate due to the rapid decrease of initial estimation error as  $T$  increases.

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**Algorithm 4** Deterministic static (DS)

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- 1: **Input:**  $p \in (0, 1), T \geq 0$ .
  - 2: **Allocation:** Run  $N_1 = \lfloor pT \rfloor$  and  $N_2 = \lfloor (1 - p)T \rfloor$  replications for designs 1 and 2.
  - 3: **Output:**  $\arg \max_{i \in \{1, 2\}} \bar{X}_{i, N_i}$ .
- 

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**Algorithm 5** Randomized static (RS)

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- 1: **Input:**  $p \in (0, 1), T \geq 0$ .
  - 2: **Allocation:** At each iteration, independently simulate design 1 with probability  $p$ , and design 2 with probability  $1 - p$ .
  - 3: **Output:**  $\arg \max_{i \in \{1, 2\}} \bar{X}_{i, N_i}$ .
- 

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**Algorithm 6** Two-phase

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- 1: **Input:**  $\alpha_0 \in (0, 1), T \geq 0$ .
  - 2: **Phase I:** Run  $N_0 = \lfloor \alpha_0 T / 2 \rfloor$  replications for each design and compute  $S_{1, N_0}$  and  $S_{2, N_0}$ . Set  $\hat{p} \leftarrow S_{1, N_0} / (S_{1, N_0} + S_{2, N_0})$ .
  - 3: **Phase II:** Run  $N_1 = \lfloor (1 - \alpha_0) \hat{p} T \rfloor$  additional replications from design 1, and  $N_2 = \lfloor (1 - \alpha_0)(1 - \hat{p}) T \rfloor$  additional replications from design 2.
  - 4: **Output:**  $\arg \max_{i \in \{1, 2\}} \bar{X}_{i, N_i}$ .
-

### 3.3.2 Analysis of DS Algorithm

Before proceeding to the LD rate analysis of the RS and two-phase algorithms, we recall some well-established results for the DS algorithm. In addition, we also derive a few new results which will serve as benchmarks. Following the normality assumption and letting  $\delta := \mu_1 - \mu_2$ , the PFS can be written as

$$\text{PFS}_{\text{DS}}(T) = \mathbb{P}(\bar{X}_{1,N_1} - \bar{X}_{2,N_2} < 0) = \int_{-\infty}^{-\frac{\delta}{\sqrt{\frac{\sigma_1^2}{N_1} + \frac{\sigma_2^2}{N_2}}}} \frac{1}{\sqrt{2\pi}} e^{-\frac{t^2}{2}} dt,$$

where we assume that  $\mu_1 > \mu_2$  and  $\sigma_1, \sigma_2 > 0$  henceforth. Ignoring the integrality constraints on  $N_1$  and  $N_2$ , it can be shown that setting  $N_1/(N_1 + N_2) \approx p^* := \sigma_1/(\sigma_1 + \sigma_2)$  minimizes the PFS. In simulation literature, this is often known as “the optimal strategy for two-design problems is to allocate the budget proportionally to their standard deviations”. The same conclusion can be reached by maximizing the following LD rate with respect to  $p \in (0, 1)$ ,

$$-\lim_{T \rightarrow \infty} \frac{1}{T} \log \text{PFS}_{\text{DS}}(T) = \frac{\delta^2}{2 \left( \frac{\sigma_1^2}{p} + \frac{\sigma_2^2}{1-p} \right)},$$

where  $p^*$  is again the unique maximizer, and the corresponding optimal LD rate is given by

$$R_{\text{DS}}^*(\delta, \sigma_1, \sigma_2) := \frac{\delta^2}{2(\sigma_1 + \sigma_2)^2}. \quad (3.3.1)$$

We will use the optimal DS allocation as a benchmark in subsequent analysis. In practice, the true variances are unknown and thus  $p^*$  cannot be implemented. A simple alternative is equal allocation (EA), i.e., setting  $p = 1/2$ . The LD rate for EA is given by

$$R_{\text{EA}}(\delta, \sigma_1, \sigma_2) := \frac{\delta^2}{4(\sigma_1^2 + \sigma_2^2)}. \quad (3.3.2)$$

Since  $2(\sigma_1 + \sigma_2)^2 \leq 4(\sigma_1^2 + \sigma_2^2) \leq 4(\sigma_1 + \sigma_2)^2$ , we have  $R_{\text{DS}}^*/2 \leq R_{\text{EA}} \leq R_{\text{DS}}^*$ . In other words, EA’s LD rate is never more than a factor of 2 away from the optimal DS rate.



Another interesting fact is that, without prior knowledge on the designs' performance, EA is the most robust algorithm. Indeed, consider the robust optimization problem

$$\inf_{p \in [0,1]} \sup_{\sigma_1, \sigma_2 > 0} \left\{ \frac{R^*(\delta, \sigma_1, \sigma_2)}{R_{\text{EA}}(\delta, \sigma_1, \sigma_2)} = \frac{\frac{\sigma_1^2}{p} + \frac{\sigma_2^2}{1-p}}{(\sigma_1 + \sigma_2)^2} \right\},$$

which is to find the  $p$  that minimizes the worst case ratio between  $R_{\text{DS}}^*$  and  $R_{\text{EA}}$ . It can be checked that the inner-layer problem's optimal value is  $\min\{\frac{1}{p}, \frac{1}{1-p}\}$ , so  $p = 1/2$  is the optimal solution.

We now derive a PFS bound that holds for an important class of algorithms. Since the optimal DS allocation only involves the designs' variance information, it would be reasonable for us to restrict our discussion to algorithms with the following property.

**Definition 3.3.1.** *A fully sequential algorithm is called variance-driven if*

- (i) *at iteration  $\ell = 0$ , it runs  $N_0 \geq 2$  replications for each design to obtain initial variance estimates  $S_1^2(0)$  and  $S_2^2(0)$ ;*
- (ii) *at every iteration  $\ell = \bar{\ell}$ , the algorithm decides which design to simulate next solely based on  $(S_1^2(\ell), S_2^2(\ell))$  for all  $\ell \leq \bar{\ell}$ , i.e., the history of variance estimates up to iteration  $\bar{\ell}$ ;*
- (iii) *at the end of final iteration  $\ell = L$ , output  $\hat{b} = \arg \max_{i \in \{1,2\}} \bar{X}_{i, N_i(L)}$ .*

Note that in the case of  $K = 2$ , OCBA's allocation fractions in (3.2.2) degenerate to  $\alpha_1/\alpha_2 = \sigma_1/\sigma_2$ . Therefore, the three OCBA-type algorithms we considered in Section 3.2, i.e., OCBA, OCBA-D and OCBA-R, all fall into the category of variance-driven on two-design problems. We will derive a tight PFS upper bound which holds for all algorithms of this type.

**Lemma 3.3.1.** *Let  $\bar{X}_n$  and  $S_n^2$  be the sample mean and sample variance of  $n$  i.i.d. normal random variables, respectively. Then, for all  $n \geq 2$ ,  $\bar{X}_n$  is independent of  $(S_2^2, S_3^2, \dots, S_n^2)$ .*

*Proof of Lemma 3.3.1.* For any  $2 \leq k \leq n$ ,  $S_k^2$  is a function of the deviations  $(\bar{X}_k - X_1, \dots, \bar{X}_k - X_k)$ . Thus, it suffices to show that

$$\bar{X}_n \perp\!\!\!\perp ((\bar{X}_2 - X_1, \bar{X}_2 - X_2), \dots, (\bar{X}_n - X_1, \dots, \bar{X}_n - X_n)),$$

where  $\perp\!\!\!\perp$  denotes independence, and we denote the RHS by  $Y_n$ . Note that  $(\bar{X}_n, Y_n)$  is a linear transformation of  $(X_1, \dots, X_n)$  and hence are jointly normal, the result follows from

$$\text{Cov}(\bar{X}_n, \bar{X}_k - X_j) = 0, \quad \forall 2 \leq k \leq n, j \leq k,$$

which can be checked by direct computation.  $\square$

Lemma 3.3.1 is an extension of the well-known result that  $\bar{X}_n$  and  $S_n^2$  are independent for normal distribution. Given a total budget of  $T$ , we let  $N_1$  and  $N_2$  denote the total number of simulation runs for designs 1 and 2 when the algorithm terminates, i.e.,  $N_1 + N_2 = T$ . Then, Lemma 3.3.1 has the following implication in our context.

**Corollary 3.3.1.** *For any variance-driven algorithm, it holds that  $(\bar{X}_{1,N_1}, \bar{X}_{2,N_2}) \mid N_1 \sim (Z_1, Z_2)$  almost surely, where  $Z_1 \sim \mathcal{N}(\mu_1, \sigma_1^2/N_1)$ ,  $Z_2 \sim \mathcal{N}(\mu_2, \sigma_2^2/(T - N_1))$ , and  $Z_1$  is independent of  $Z_2$ .*

*Proof of Corollary 3.3.1.* For  $N_0 \leq k \leq T - N_0$ , let

$$Y_{1,k} := (S_{1,N_0}, \dots, S_{1,k}), \quad Y_{2,k} := (S_{2,N_0}, \dots, S_{2,k}).$$

Note that  $N_1 = k$  if and only if  $(Y_{1,k}, Y_{2,T-k})$  falls into some event  $A_k(T)$  that is measurable. Furthermore, following the proof of Lemma 3.3.1, it can be shown that  $(\bar{X}_{1,k}, \bar{X}_{2,T-k})$

$\perp\!\!\!\perp(Y_{1,k}, Y_{2,T-k})$  since  $(X_{1,1}, X_{1,2}, \dots) \perp\!\!\!\perp (X_{2,1}, X_{2,2}, \dots)$ . Thus, for any  $N_0 \leq k \leq T - N_0$ ,

$$\begin{aligned} & \mathbb{P}(\bar{X}_{1,N_1} \leq x, \bar{X}_{2,N_2} \leq y \mid N_1 = k) \\ &= \mathbb{P}(\bar{X}_{1,k} \leq x, \bar{X}_{2,T-k} \leq y \mid (Y_{1,k}, Y_{2,T-k} \in A_k(T))) \\ &= \mathbb{P}(\bar{X}_{1,k} \leq x, \bar{X}_{2,T-k} \leq y). \end{aligned}$$

The conclusion follows from  $\bar{X}_{1,k} \perp\!\!\!\perp \bar{X}_{2,T-k}$ .  $\square$

Generally speaking, the final mean estimates  $\bar{X}_{1,N_1}$  and  $\bar{X}_{2,N_2}$  can have a highly non-trivial correlation if an algorithm sequentially allocates the computing budget based on some iteratively updated statistics. Surprisingly, Corollary 3.3.1 reveals that for variance-driven algorithms,  $\bar{X}_{1,N_1}$  and  $\bar{X}_{2,N_2}$  are conditionally independent given  $N_1 = n_1$  for some  $n_1 \geq N_0$ . Moreover, their joint distribution coincides with what we get from deterministically allocating  $n_1$  and  $T - n_1$  runs to designs 1 and 2, respectively. This is due to the nice property of normal distribution characterized in Lemma 3.3.1, and it gives rise to a tight PFS lower bound for all variance-driven algorithms.

**Proposition 3.3.1.** *For any variance-driven algorithm  $\mathcal{A}$ , we have*

$$PFS_{\mathcal{A}}(T) \geq 1 - \Phi\left(\frac{\delta\sqrt{T}}{\sigma_1 + \sigma_2}\right), \quad \forall T \geq 2N_0,$$

where  $\Phi$  is the cumulative distribution function (c.d.f.) of  $\mathcal{N}(0, 1)$  distribution.

*Proof of Proposition 3.3.1.* For any fixed  $N_0 \leq N_1 \leq T - N_0$ ,

$$\text{PFS} = \mathbb{P}(\bar{X}_{1,N_1} < \bar{X}_{2,T-N_1}) = 1 - \Phi\left(\frac{\delta}{\sqrt{\frac{\sigma_1^2}{N_1} + \frac{\sigma_2^2}{T-N_1}}}\right),$$

where the right-hand side (RHS) is convex in  $N_1$  and is minimized when  $N_1 = N_1^* := p^*T$ . For an algorithm  $\mathcal{A}$  described in the statement, it follows from Corollary 3.3.1 that  $(\bar{X}_{1,N_1}, \bar{X}_{2,N_2}) \mid N_1$  is distributed as two independent normal random variables. Thus, by

Jensen's inequality,

$$\text{PFS}_{\mathcal{A}}(T) = \mathbb{E} [\mathbb{P} (\bar{X}_{1,N_1} < \bar{X}_{2,N_2} \mid N_1)] \geq \mathbb{P} (\bar{X}_{1,\mathbb{E}N_1} < \bar{X}_{2,\mathbb{E}N_2}),$$

where the RHS is further bounded from below by the PFS corresponding to  $N_1^*$ , which yields exactly the lower bound in the statement.  $\square$

Proposition 3.3.1 establishes optimality for the optimal DS algorithm in a very strong sense: no variance-driven algorithm can beat the optimal DS allocation under any finite  $T$  (up to some rounding error). The same typically does not hold if  $K \geq 3$ , where it can be checked numerically that the optimal DS algorithm may perform poorly on some problem instances under small budgets. Nonetheless, from an asymptotic point of view, it remains an open question whether sequential algorithms can achieve a higher LD rate than the optimal DS algorithm when  $K \geq 3$ .

### 3.3.3 Analysis of RS Algorithm

Recall from Algorithm 5 that at each iteration, the RS algorithm simulates design 1 with probability (w.p.)  $p$  and design 2 w.p.  $1 - p$ , where  $p \in (0, 1)$  and the samples are independent of the decisions. Let  $\{U(\ell)\}$  be a sequence of i.i.d. Bernoulli( $p$ ) random variables representing whether design 1 is sampled at each iteration  $\ell$ . To ensure that the sample means are well-defined, we set  $N_1 = \sum_{\ell=1}^T U(\ell) + 1$ ,  $N_2 = T - N_1 + 1$  so that each design gets sampled at least once. Then, the PFS is given by

$$\begin{aligned} \text{PFS}_{\text{RS}}(T) &= \mathbb{P}(\bar{X}_{1,N_1} < \bar{X}_{2,N_2}) = \mathbb{E}[\mathbb{P}(\bar{X}_{1,N_1} < \bar{X}_{2,N_2} \mid N_1)] \\ &= \sum_{k=0}^T \mathbb{P}(\bar{X}_{1,k+1} < \bar{X}_{2,(T-k)+1}) \binom{n}{k} p^k (1-p)^{T-k}, \end{aligned} \quad (3.3.3)$$

which does not allow a closed form. However, a quick observation is that the RHS of (3.3.3) is bounded from below by the term corresponding to  $k = 0$ , i.e.,

$$\text{PFS}_{\text{RS}}(T) \geq \mathbb{P}(\bar{X}_{1,1} < \bar{X}_{2,T+1}) (1-p)^T, \quad \forall T,$$

which gives the LD rate upper bound

$$-\lim_{T \rightarrow \infty} \frac{1}{T} \log \text{PFS}_{\text{RS}}(T) \leq -\log(1-p).$$

Thus, the RS algorithm's LD rate is bounded as  $\delta \rightarrow \infty$ , which is in sharp contrast with the LD rate of the DS algorithm, where the latter grows in order  $\delta^2$  according to (3.3.1). Since the separation margin of  $\mu_1$  and  $\mu_2$  measures the difficulty of a correct selection, this means that the RS algorithms cannot take advantage of a larger  $\delta$  due to the randomness introduced in allocation. It also echoes our observation in Section 3.2 that algorithms with the same limiting allocation fractions may have drastically different LD rates. More precisely, we have the following exact characterization.

**Theorem 3.3.1.** *For the RS algorithm, we have*

$$-\lim_{T \rightarrow \infty} \frac{1}{T} \log \text{PFS}_{\text{RS}}(T) = \inf_{\alpha \in [0,1]} \left\{ \frac{\delta^2}{2 \left( \frac{\sigma_1^2}{\alpha} + \frac{\sigma_2^2}{1-\alpha} \right)} + kl(\alpha, p) \right\}, \quad (3.3.4)$$

where  $kl(\alpha, p) := \alpha \log \frac{\alpha}{p} + (1-\alpha) \log \frac{1-\alpha}{1-p}$  is the Kullback-Leibler (K-L) divergence between two Bernoulli distributions with parameters  $\alpha$  and  $p$ , respectively.

The optimization problem in (3.3.4) is in general non-convex and an analytical solution is not available. Nonetheless, it can be checked numerically that the  $p$  value maximizing the LD rate of the RS algorithm is different from  $p^*$ , the optimal DS fraction. The proof of Theorem 3.3.1 relies on the following lemma, where  $\mathbb{Z}^+$  denotes the set of nonnegative integers.

**Lemma 3.3.2.** Let  $g_T : \mathbb{Z}^+ \mapsto (0, \infty)$  be a sequence of functions for  $T \in \mathbb{Z}^+$ . If there exists a function  $g^* : (0, 1) \mapsto \mathbb{R}$  such that  $\frac{1}{T} \log g_T(\lfloor \alpha T \rfloor)$  converges uniformly to  $g^*(\alpha)$  on  $\alpha \in [0, 1]$ , then

$$\lim_{T \rightarrow \infty} \frac{1}{T} \log \left[ \sum_{k=0}^T g_T(k) \right] = \sup_{\alpha \in [0, 1]} g^*(\alpha). \quad (3.3.5)$$

*Proof of Lemma 3.3.2.* First of all, notice that

$$\lim_{T \rightarrow \infty} \frac{1}{T} \log \left[ \sum_{k=0}^T g_T(k) \right] \geq \lim_{T \rightarrow \infty} \frac{1}{T} \log g_T(\lfloor \alpha T \rfloor) = g^*(\alpha), \quad \forall \alpha \in [0, 1].$$

so taking the supremum on the RHS gives a lower bound. For the upper bound,

$$\begin{aligned} \lim_{T \rightarrow \infty} \frac{1}{T} \log \left[ \sum_{k=0}^T g_T(k) \right] &\leq \lim_{T \rightarrow \infty} \sup_{\alpha \in [0, 1]} \frac{1}{T} \log [(T+1)g_T(\lfloor \alpha T \rfloor)] \\ &= \sup_{\alpha \in [0, 1]} \lim_{T \rightarrow \infty} \log \frac{1}{T} [(T+1)g_T(\lfloor \alpha T \rfloor)] \\ &= \sup_{\alpha \in [0, 1]} g^*(\alpha), \end{aligned}$$

where the interchange of limit and supremum is justified by the uniform convergence of  $\frac{1}{T} \log g_T(\lfloor \alpha T \rfloor)$  (see, e.g., Theorem 5.3 in [67]).  $\square$

Lemma 3.3.2 can be viewed as a generalization of  $\lim_{t \rightarrow \infty} \frac{1}{t} \log(e^{-at} + e^{-bt}) = b$  for  $a > b > 0$ , i.e., the LD rate of a sum is determined by the largest summand. In the context of Theorem 3.3.1,  $g_T(\cdot)$  is a sequence of functions that take values in  $(0, 1)$ , so (3.3.5) roughly corresponds to the  $g_T(\lfloor \alpha T \rfloor)$  term that converges to 0 “at the slowest rate”. With Lemma 3.3.2, Theorem 3.3.1 can be shown by checking the uniform convergence of the function sequence  $\frac{1}{T} \log g_T(\lfloor \alpha T \rfloor)$ .

*Proof of Theorem 3.3.1.* Recall the following Gaussian tail bound. For  $X \sim \mathcal{N}(0, 1)$  and  $x > 0$ ,

$$e^{-\frac{x^2}{2}} \geq \mathbb{P}(X > x) \geq \frac{x}{x^2 + 1} \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}. \quad (3.3.6)$$

Applying the upper bound in (3.3.6) to the PFS expression in (3.3.3) yields

$$\text{PFS}_{\text{RS}}(T) \leq \sum_{k=0}^T \exp \left( -\frac{\delta^2}{2 \left( \frac{\sigma_1^2}{k+1} + \frac{\sigma_2^2}{T-k+1} \right)} \right) \binom{n}{k} p^k (1-p)^{T-k}. \quad (3.3.7)$$

We will apply Lemma 3.3.2 to (3.3.7) to show a lower bound for the RS algorithm's LD rate. The upper bound follows similarly from the lower bound in (3.3.6) and is thus omitted.

Letting  $g_T(k)$  denote the summands in the RHS of (3.3.7), we have

$$\begin{aligned} \frac{1}{T} \log g_T(\lfloor \alpha T \rfloor) = & \left\{ -\frac{\delta^2}{2 \left( \frac{\sigma_1^2 T}{\lfloor \alpha T \rfloor + 1} + \frac{\sigma_2^2 T}{\lfloor (1-\alpha)T \rfloor + 1} + 1 \right)} \right. \\ & + \frac{1}{T} \log \left( \frac{\Gamma(T+1)}{\Gamma(\lfloor \alpha T \rfloor + 1) \Gamma(\lfloor (1-\alpha)T \rfloor + 1)} \right) \\ & \left. + \frac{1}{T} \log (p^{\lfloor \alpha T \rfloor}) + \frac{1}{T} \log [(1-p)^{\lfloor (1-\alpha)T \rfloor}] \right\}, \end{aligned} \quad (3.3.8)$$

where the first, third and fourth terms are clearly uniformly convergent in  $\alpha$  as  $T \rightarrow \infty$ . For the second term, a well-known approximation of the log gamma function (see, e.g., [82, 83]) gives

$$\log \Gamma(x) = \left( x - \frac{1}{2} \right) \log x - x + \frac{1}{2} \log(2\pi) + r(x), \quad (3.3.9)$$

where there exists a constant  $C > 0$  such that the remainder  $|r(x)| < C/x$  for all  $x \geq 1$ . It follows from (3.3.9) that the second term converges uniformly to  $-\alpha \log \alpha - (1-\alpha) \log(1-\alpha)$ . Sending  $T \rightarrow \infty$  in (3.3.8) gives the objective function in the RHS of (3.3.4), and applying Lemma 3.3.2 leads to the infimum problem.  $\square$

### 3.3.4 Analysis of Two-phase Algorithm

Recall from Algorithm 6 that the two-phase algorithm first uses  $\alpha_0$  fraction of the budget to obtain initial estimates of  $\sigma_1$  and  $\sigma_2$ , and then allocates the remaining budget according to the plug-in estimate of  $p^*$  given by  $\hat{p} := S_1/(S_1 + S_2)$ . Since the allocation in phase II only

depends on the value of  $\hat{p}$  from phase I, we first characterize  $\hat{p}$ 's distribution as follows.

**Lemma 3.3.3.** *The probability density function (p.d.f.) of  $\hat{p}$  is given by*

$$f_{N_0}(p) = \frac{2\Gamma(N_0 - 1)}{[\Gamma(\frac{N_0-1}{2})]^2} [p(1-p)]^{N_0-2} \left( \frac{\sigma_1\sigma_2}{(1-p)^2\sigma_1^2 + p^2\sigma_2^2} \right)^{N_0-1}, \quad p \in [0, 1],$$

where  $\Gamma$  is the gamma function  $\Gamma(t) = \int_0^\infty x^{t-1}e^{-x}dx$ .

*Proof of Lemma 3.3.3.* Given two independent nonnegative random variables  $X, Y$  with probability densities functions (p.d.f.s)  $f_X$  and  $f_Y$ , it can be verified that for  $t \in (0, 1)$ ,

$$\frac{d}{dt} \mathbb{P} \left( \frac{X}{X+Y} \leq t \right) = \frac{1}{(1-t)^2} \int_0^\infty y f_X \left( \frac{t}{1-t} y \right) f_Y(y) dy. \quad (3.3.10)$$

So we only need to compute the p.d.f.s for  $S_1$  and  $S_2$ . Suppose that  $N_0 = n$ . Then, since  $(n-1)S_1^2/\sigma_1^2 \sim \chi^2(n-1)$ ,

$$\mathbb{P}(S_1 \leq x) = \mathbb{P} \left( \chi^2(n-1) \leq \frac{(n-1)x^2}{\sigma_1^2} \right),$$

and by differentiating on both sides,

$$f_{S_1}(x) = \frac{2(n-1)x}{\sigma_1^2 2^{\frac{n-1}{2}} \Gamma(\frac{n-1}{2})} \left( \frac{(n-1)x^2}{\sigma_1^2} \right)^{\frac{n-3}{2}} \exp \left( -\frac{(n-1)x^2}{2\sigma_1^2} \right).$$

The p.d.f. of  $S_2$  has a similar form and is omitted. Plugging their densities into (3.3.10) and a direct computation yields the result.  $\square$

With Lemma 3.3.3, we can apply a similar technique involving “the slowest term” in Section 3.3.3 to establish the LD rate of the two-phase algorithm.



**Theorem 3.3.2.** *For the two-phase algorithm, we have*

$$-\lim_{T \rightarrow \infty} \frac{1}{T} \log \text{PFS}(T) = \min_{p \in [0,1]} \left\{ \frac{(1-\alpha_0)\delta^2}{2\left(\frac{\sigma_1^2}{p} + \frac{\sigma_2^2}{1-p}\right)} + \frac{\alpha_0}{2} \log \left( \frac{(1-p)^2\sigma_1^2 + p^2\sigma_2^2}{2p(1-p)\sigma_1\sigma_2} \right) \right\}. \quad (3.3.11)$$

*Proof of Theorem 3.3.2.* The PFS for the two-phase algorithm is given by

$$\int_0^1 \mathbb{P} \left( \mathcal{N} \left( \delta, \frac{\sigma_1^2}{\lfloor (1-\alpha_0)pT \rfloor + 1} + \frac{\sigma_2^2}{\lfloor (1-\alpha_0)(1-p)T \rfloor + 1} \right) < 0 \right) f_{N_0}(p) dp. \quad (3.3.12)$$

Apply the Gaussian tail bounds in (3.3.6) and we have

$$\int_0^1 \psi_T(p) f_{N_0}(p) dp \geq \text{PFS}(T) \geq K(T) \int_0^1 \psi_T(p) f_{N_0}(p) dp, \quad (3.3.13)$$

where the function  $\psi_T$  is defined as

$$\psi_T(p) := \exp \left\{ - \frac{\delta^2}{2 \left( \frac{\sigma_1^2}{\lfloor (1-\alpha_0)pT \rfloor + 1} + \frac{\sigma_2^2}{\lfloor (1-\alpha_0)(1-p)T \rfloor + 1} \right)} \right\},$$

and  $K(T)$  is of order  $\sqrt{T}$  as  $T \rightarrow \infty$ . From (3.3.13) we know that the PFS has the same LD rate as  $\int_0^1 \psi_T(p) f_{N_0}(p) dp$ , so it suffices to study the latter. Similar to the proof of Theorem 3.3.1, if  $g_T(p) := \frac{1}{T} \log (\psi_T(p) f_{N_0}(p))$  converges uniformly to a function  $g^*$  on  $p \in [0, 1]$  as  $T \rightarrow \infty$ , then Theorem 5.3 in [67] guarantees that

$$\lim_{T \rightarrow \infty} \max_{p \in [0,1]} g_T(p) = \max_{p \in [0,1]} g^*(p). \quad (3.3.14)$$

To check uniform convergence, we have

$$\begin{aligned}
g_T(p) = & \underbrace{-\frac{\delta^2}{2T \left( \frac{\sigma_1^2}{\lfloor (1-\alpha_0)pT \rfloor + 1} + \frac{\sigma_2^2}{\lfloor (1-\alpha_0)(1-p)T \rfloor + 1} \right)}}_{(1)} + \underbrace{\frac{N_0 - 2}{T} \log(p(1-p))}_{(2)} \\
& + \underbrace{\frac{N_0 - 1}{T} \log(\sigma_1 \sigma_2 / [(1-p)^2 \sigma_1^2 + p^2 \sigma_2^2])}_{(3)} + \underbrace{\frac{1}{T} \log \left( \frac{2\Gamma(N_0 - 1)}{[\Gamma(\frac{N_0 - 1}{2})]^2} \right)}_{(4)},
\end{aligned}$$

where  $N_0 = \lfloor \alpha_0 T / 2 \rfloor$  and  $-\lim_{T \rightarrow \infty} g_T(p)$  gives the objective function in the RHS of (3.3.11). The uniform convergence of (1), (3) and (4) can be easily checked. However, (2) is not uniformly convergent near the two endpoints 0 and 1. To show (3.3.14), note that (1), (3) and (4) are all uniformly bounded in  $p$  and  $T$ , while  $\log(p(1-p)) \rightarrow -\infty$  as  $p \rightarrow 0$  or 1. Thus, for any  $M > 0$  and  $\epsilon > 0$ , there exists corresponding  $0 < p_1 < p_2 < 1$  such that for all  $T$  large enough,

$$g_T(p) < M - \epsilon, \quad \forall p \in [0, p_1) \cup (p_2, 1]. \quad (3.3.15)$$

Fix a  $\tilde{p} \in (0, 1)$  and take  $M = g^*(\tilde{p})$ . Then,  $g_T(\tilde{p}) \geq M - \epsilon$  for all  $T$  large enough, which together with (3.3.15) implies that the maximizer of  $g_T$  can only lie in  $[p_1, p_2]$  for all  $T$  large. Let  $p^* \in \arg \max_{p \in [0, 1]} g^*(p)$ , which is guaranteed to exist since  $g^*$  is continuous on  $(0, 1)$  and  $g^*(p) \rightarrow -\infty$  as  $p \rightarrow 0$  or 1 (see, e.g., Proposition A.8 in [84] for Weierstrass' Extreme Value Theorem). Further expand the interval  $[p_1, p_2]$  if necessary such that  $p^* \in [p_1, p_2]$ , which does not affect the preceding argument. Since  $g_T$  converges uniformly on  $[p_1, p_2]$ ,

we have

$$\begin{aligned}
\lim_{T \rightarrow \infty} \frac{1}{T} \log \int_0^1 (\psi_T(p) f_{N_0}(p)) dp &\leq \lim_{T \rightarrow \infty} \frac{1}{T} \log \left( \max_{p \in [p_1, p_2]} \psi_T(p) f_{N_0}(p) \right) \\
&\leq \lim_{T \rightarrow \infty} \max_{p \in [p_1, p_2]} g_T(p) \\
&= \max_{p \in [p_1, p_2]} g^*(p) = \max_{p \in [0, 1]} g^*(p),
\end{aligned}$$

where the last equality follows from  $p^* \in [p_1, p_2]$ . For a lower bound, choose an  $\epsilon > 0$  such that  $[p^* - \epsilon, p^* + \epsilon] \subseteq [0, 1]$ , and we have

$$\begin{aligned}
\lim_{T \rightarrow \infty} \frac{1}{T} \log \int_0^1 (\psi_T(p) f_{N_0}(p)) dp &\geq \lim_{T \rightarrow \infty} \frac{1}{T} \log \int_{p^* - \epsilon}^{p^* + \epsilon} (\psi_T(p) f_{N_0}(p)) dp \\
&\geq \lim_{T \rightarrow \infty} \min_{p \in [p^* - \epsilon, p^* + \epsilon]} \frac{1}{T} \log (2\epsilon \psi_T(p) f_{N_0}(p)) \\
&= \min_{p \in [p^* - \epsilon, p^* + \epsilon]} g^*(p),
\end{aligned}$$

where the last equality is due to uniform convergence. Take  $\epsilon \downarrow 0$  and the lower bound follows from the continuity of  $g^*$  on  $(0, 1)$ .  $\square$

We argue that the RHS of (3.3.11) is not bounded in  $\delta$ . Let  $p_\delta^*$  be the minimizer corresponding to parameter  $\delta$ , and let  $\underline{p}^* := \liminf_{\delta \rightarrow \infty} p_\delta^*$ ,  $\bar{p}^* := \limsup_{\delta \rightarrow \infty} p_\delta^*$ . If  $\underline{p}^* = 0$  or  $\bar{p}^* = 1$ , then the second term in the objective function is unbounded in  $\delta$ ; otherwise if  $\underline{p}^* > 0$  and  $\bar{p}^* < 1$ , then the first term will be unbounded as  $\delta \rightarrow \infty$ . Either case, the two-phase algorithm does not suffer from an LD rate bottleneck as the RS algorithm does. However, it can be checked numerically that the two-phase algorithm is usually far from matching the LD rate of the optimal DS algorithm. This should be no surprise since  $\hat{p}$  is subject to estimation error.

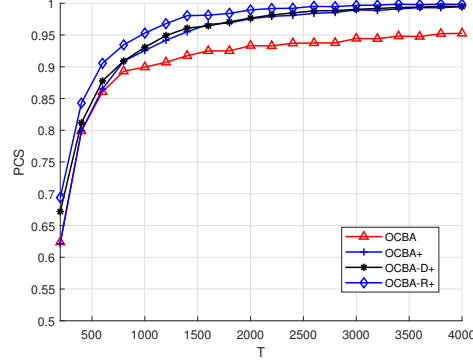
### 3.4 Numerical Results

We test the performance of four algorithms: OCBA, OCBA+, OCBA-D+, OCBA-R+, where OCBA is the original OCBA with a constant initial sample size  $N_0$ , and the “+” algorithms are modified versions that implement  $N_0 = \lfloor \alpha_0 T \rfloor$  for some chosen  $\alpha_0 \in (0, 1)$ . The purpose is to see whether making  $N_0$  grow linearly with  $T$  can boost the PCS. We apply these algorithms to six problem instances, which are listed as follows. In particular, the “Slippage Configuration” refers to the least favorable setting where all the suboptimal designs have the same mean.

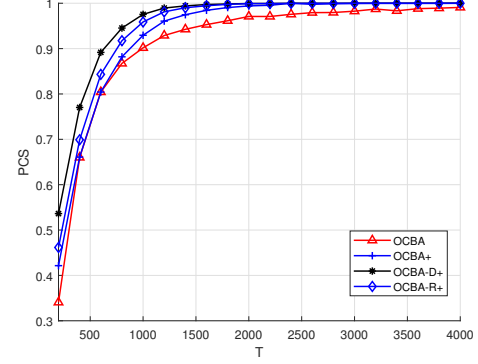
- (1) *Ten designs A*:  $\mu = [1, 1.1, 1.2, \dots, 1.8, 5], \sigma = [5, 5, \dots, 5, 20]$ .
- (2) *Ten designs B*:  $\mu = [1, 1.1, 1.2, \dots, 1.8, 5], \sigma = [20, 20, \dots, 20, 5]$ .
- (3) *Slippage Configuration A*:  $\mu = [1, 1, 1, 1, 2], \sigma = [2, 2, 2, 2, 10]$ .
- (4) *Slippage Configuration B*:  $\mu = [1, 1, 1, 1, 2], \sigma = [10, 10, 10, 10, 2]$ .
- (5) *Equal variances*:  $\mu = [1, 2, \dots, 10], \sigma_i = 10, \forall i = 1, 2, \dots, 10$ .
- (6) *Increasing variances*:  $\mu = [1, 2, \dots, 10], \sigma = [6, 7, 8, \dots, 15]$ .

The algorithm parameters are  $N_0 = 10, \Delta = 20$  for OCBA, and  $\alpha_0 = 0.2$  for all the modified algorithms. We would like to see how fast the PCS converges to 1 as  $T$  increases from 200 to 4000 (with an increment of 200). To estimate the PCS, all the algorithms are run for 10,000 independent replications using common random numbers, i.e., the algorithms share the same  $X_{ir}$  samples for each design. The PCS curves are gathered in Figure 3.1, and a number of observations follow.

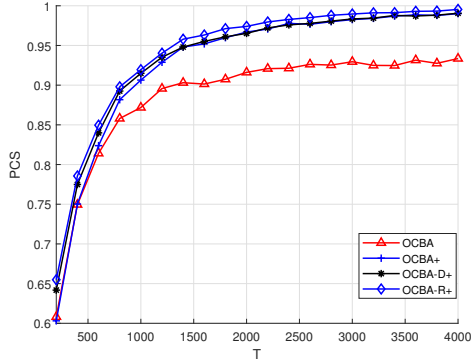
1. In Figure 3.1 (a)-(f), the modified algorithms achieve a higher PCS than OCBA for every fixed  $T$ . This demonstrates the advantage of using a linearly growing  $N_0$ .



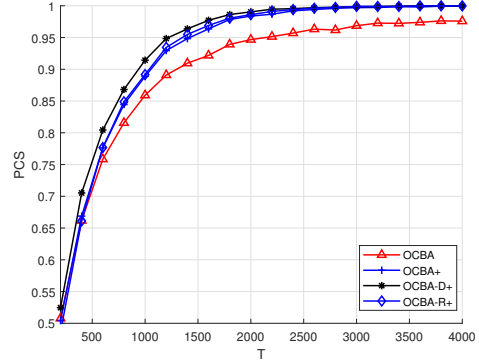
(a) Ten designs A.



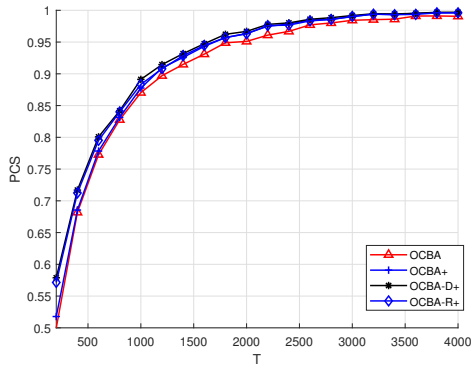
(b) Ten designs B.



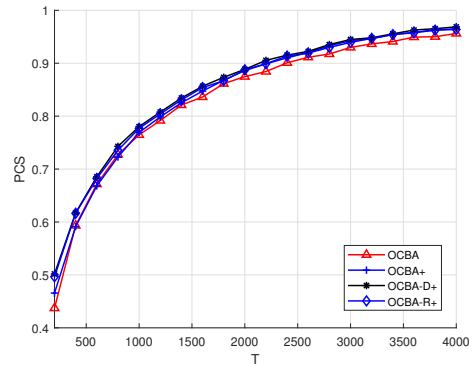
(c) Slippage Configuration A.



(d) Slippage Configuration B.



(e) Equal variances.



(f) Increasing variances.

Figure 3.1: Comparison of PCS for different algorithms.

2. In Figure 3.1 (a) and (c), OCBA clearly suffers from slower convergence. Notably, on those two problem instances, OCBA takes approximately three times the budget of OCBA-R+ to attain a 95% PCS, which echoes our finding that a constant  $N_0$  only gives a polynomial rate.
3. The improvement is less visible in Figure 3.1 (e) and (f), where the corresponding instances are “easier” as they have relatively spread-out means and smaller variances. Therefore, more benefit can be gained from using linearly growing  $N_0$  on “harder” problem instances.
4. Among the modified algorithms, OCBA-D+ and OCBA-R+ outperform OCBA+ on all problem instances, which can be expected from their fully sequential feature as it makes better use of the budget. However, no clear ranking is observed between OCBA-D+ and OCBA-R+.

### 3.5 Conclusion and Future Work

This chapter studies the problem of fixed budget Ranking and Selection with independent normal samples. By analyzing the performance of several OCBA-type algorithms, we discover that a budget-independent initial sample size only leads to a sub-exponential convergence rate. A linearly growing initial sample size is then proposed to achieve both better theoretical (asymptotic) and practical (finite-sample) performance. In addition, we explicitly characterize the large deviations rate of some simplified algorithms, which sets a basis for more general convergence analysis.

With the study of fixed budget Ranking and Selection actively ongoing, we think that this work points to a least a number of directions that are worth pursuing.

1. *Tighter PFS bounds.* Our chapter explores some techniques for analyzing the convergence rate of sequential allocation algorithms. However, more powerful approaches

still need to be developed to derive tighter PFS bounds which capture the features of different algorithms.

2. *Explicit balance between exploration and exploitation.* The fixed budget Ranking and Selection problem is also called a “pure exploration” problem in the Multi-Armed Bandits literature, as the tradeoff between exploration and exploitation is relatively less explicit. It would be practically useful to design an algorithm that can explicitly balance these two aspects.
3. *Better performance measure.* As is mentioned at the end of Section 3.1, the three prevailing performance measures, i.e., finite-sample bounds, large deviations rate and numerical results, are all subject to some restrictions. This calls for a better performance measure, which should not only reflect the general performance of algorithms, but also allow tractable characterization.

## CHAPTER 4

### RANKING AND SELECTION UNDER INPUT UNCERTAINTY: FIXED CONFIDENCE AND FIXED BUDGET

In this chapter, we study R&S in the presence of IU. Different from Chapter 2, here we assume that additional data can be collected to reduced IU. Two classical frameworks, fixed confidence and fixed budget, are extended to this setting, and new algorithms are proposed to solve the formulated optimization problems.

The rest of the chapter is organized as follows. The basic settings and notations are reviewed in Section 4.1. Sections 4.2 and 4.3 introduce the fixed confidence and fixed budget formulations, respectively, with corresponding algorithms developed along the way. After that, we present the numerical results in Section 4.4, and conclude in Section 4.5.

#### 4.1 Basic Settings

The R&S problem we study is concerned with identifying the design with the highest expected performance among  $K$  alternatives. Denote by  $\mathcal{I} := \{1, 2, \dots, K\}$  the enumeration of all designs. For a design  $i \in \mathcal{I}$ , let  $h_i : \mathbb{R}^m \rightarrow \mathbb{R}$  be its performance measure function, and let  $\xi \in \mathbb{R}^m$  be a random vector capturing the stochasticity in the system. Similar to [56], we study a case where all  $K$  designs share the same input distribution  $P^c$  (“c” means “correct”). The best design is defined as

$$b := \arg \max_{i \in \mathcal{I}} \mathbb{E}_{P^c}[h_i(\xi)],$$

where the expectation is assumed to be finite. We will assume that  $b$  is unique to avoid technicality. Furthermore, we make some specific assumptions on the structure of  $P^c$ . Suppose that  $P^c$  consists of several mutually independent distributions, where each input



distribution belongs to a known parametric family but with unknown parameter. More precisely, we lay down the following notations to facilitate further discussion.

- (i) We have  $Q$  mutually independent input distributions  $\{P_{\theta^c(1)}, P_{\theta^c(2)}, \dots, P_{\theta^c(Q)}\}$ , where each  $\theta^c(q)$ ,  $1 \leq q \leq Q$  lives in a closed parameter space  $\Theta(q) \subseteq \mathbb{R}^{d_q}$ .
- (ii) Then,  $P^c$  can be specified as a product measure  $P_{\theta^c} := P_{\theta^c(1)} \times \dots \times P_{\theta^c(Q)}$ , where  $\theta^c = [\theta(1)^\top, \dots, \theta(Q)^\top]^\top$  is the collection of all parameters, and  $\top$  denotes matrix transpose.
- (iii) Let  $\Theta := \prod_{q=1}^Q \Theta(q)$  and  $\sum_{q=1}^Q d_q = d$ , so  $\theta^c$  lives in a parameter space  $\Theta \subseteq \mathbb{R}^d$ .
- (iv) Similarly, we can decompose  $\xi$  into  $[\xi(1)^\top, \xi(2)^\top, \dots, \xi(Q)^\top]^\top$ , where each  $\xi(q)$ ,  $1 \leq q \leq Q$  is a random vector in  $\mathbb{R}^{m_q}$  with distribution  $P_{\theta^c(q)}$ , and  $\sum_{q=1}^Q m_q = m$ .
- (v) The input data for the the  $q$ th input distribution, denoted by  $\{\zeta_1(q), \zeta_2(q), \dots\}$ , are i.i.d. (independent and identically distributed) samples from  $P_{\theta^c(q)}$ .

For example, an M/M/1 queue simulation model has  $Q = 2$  input distributions, where  $P_{\theta^c(1)}$  is the inter-arrival time distribution, and  $P_{\theta^c(2)}$  is the service time distribution. Both distributions are exponential, with  $\theta^c(1) > 0$  and  $\theta^c(2) > 0$  being their means.

The parametric assumption on  $P^c$  can be justified by allowing a mixture of multiple parametric distributions (see the discussion in [3]), provided that the parameter space is finite-dimensional. The following notations will be used throughout the chapter.

- (i)  $H_i(\theta) := \mathbb{E}_{P_\theta}[h_i(\xi)]$ , i.e., the true performance of design  $i$  under input distribution  $P_\theta$ .
- (ii)  $\delta_{ij}(\theta) := H_i(\theta) - H_j(\theta)$ , i.e., the difference between designs  $i$  and  $j$ 's performances under input distribution  $P_\theta$ .
- (iii)  $\sigma_i^2(\theta) := \text{Var}_{P_\theta}[h_i(\xi)]$ , i.e., the variance of design  $i$ 's simulation output under input distribution  $P_\theta$ .

In traditional R&S, the true input distribution  $P_{\theta^c}$  is assumed to be known accurately, and the only source of uncertainty is SU. For a given parameter  $\theta$ , let  $\hat{H}_i(\theta)$  denote the estimate of  $H_i(\theta)$ . If design  $i$  has been simulated  $M_i$  times, then we have

$$\hat{H}_i(\theta^c) := \frac{1}{M_i} \sum_{r=1}^{M_i} h_i(\xi_{ir}), \quad \{\xi_{ir}\}_{r=1}^{M_i} \sim P_{\theta^c} \quad \text{i.i.d.}, \quad (4.1.1)$$

where the samples  $\{\xi_{ir}\}_r$  are independent across different designs unless otherwise specified. Due to the estimation error in  $\hat{H}_i(\theta^c)$ , our selected design may not be the best one. Thus, a commonly used measure of selection quality is the probability of correct selection (PCS), which is defined as

$$\text{PCS} := \mathbb{P} \left\{ b = \arg \max_{i \in \mathcal{I}} \hat{H}_i(\theta^c) \right\} = \mathbb{P} \left\{ \bigcap_{i \neq b} \left\{ \hat{\delta}_{bi}(\theta^c) > 0 \right\} \right\},$$

where  $\hat{\delta}_{ij}(\theta) := \hat{H}_i(\theta) - \hat{H}_j(\theta)$  for any two designs  $i$  and  $j$ . Informally, the two classical formulations of R&S, i.e., fixed confidence and fixed budget, are both concerned with achieving a satisfactory PCS through efficient simulation experiments. As is indicated by existing literature, R&S is already a difficult problem even without IU.

In practice, since  $\theta^c$  is usually estimated using finite real-world data, IU is inevitable and it can affect R&S adversely. To see this, consider the following set

$$\mathcal{P} := \{\theta \in \Theta \mid H_b(\theta) < \max_{i \neq b} H_i(\theta)\}, \quad (4.1.2)$$

which is the set of parameters under which the best design is perturbed into a design other than  $b$ . We will refer to  $\mathcal{P}$  as the *perturbation region*. In general,  $\mathcal{P} \neq \emptyset$  and our estimate of  $\theta^c$  can fall into  $\mathcal{P}$  with a nonzero probability. If this happens, then a suboptimal design will be selected even using infinite simulation budget (see the  $(s, S)$  inventory optimization example in [56]). Therefore, it is important to take IU into account when designing R&S algorithms. However, unlike SU, IU cannot be controlled by increasing simulation effort.

Instead, it can only be reduced by enlarging the input dataset. In what follows, we discuss how to account for IU in both the fixed confidence and the fixed budget formulations when it is possible to collect additional input data.

## 4.2 Fixed Confidence Formulation

In general, the fixed confidence formulation of R&S aims to provide a statistical selection guarantee (e.g., 95% PCS) using minimal simulation effort or other resources. In the case without IU, a large body of literature studies the IZ formulation, which allows the user to specify the smallest difference in performance worth detecting. Most IZ algorithms construct a continuation region for all pairs of designs  $(i, j)$  such that, if  $\hat{\delta}_{ij}(\theta^c)$  escapes the region, then the sign of  $\delta_{ij}(\theta^c)$  can be determined confidently based on which side  $\hat{\delta}_{ij}(\theta^c)$  exits from. Then, the key is to find a small continuation region for fast stopping without compromising the selection guarantee. Algorithms of this type include the KN algorithm [32], the BIZ algorithm [34], the IZ-free algorithms [85] among several others.

In the presence of IU, we consider a multi-stage scenario, where incremental data become available at each stage. This allows us to update the estimate of  $\theta^c$  and run further simulations to refine the estimates of  $\delta_{ij}(\theta^c)$ . With sequential input data, our goal is to deliver a PCS guarantee after a small number of “stages” (defined in Section 4.2.1). Some of the motivating examples are as follows.

- *Ride-hailing platform.* A ride hailing platform wants to use simulation to find the best price surging strategy. Some of the input models about traveling time, user behavior, route selection, etc., can be estimated using real-time data.
- *Online retailer.* An online retailer is interested in optimizing its supply chain network by comparing different ordering/inventory/fulfillment strategies through simulation. Upstream and downstream customer demand data can be collected in a timely manner to refine the demand distribution estimates.

- *Express delivery service.* An express delivery service provider intends to compare different routing and scheduling strategies via a simulation model. The input data on customer demand, traveling time, deliveryman's preference can be harvested on a daily basis.

In all of the above examples, a moderate amount of new data can be collected at a relatively low cost to continuously improve the accuracy of the simulation model. The major challenge here is that many existing algorithms cannot be extended easily to handle sequential input data. For example, most IZ algorithms rely on a normality assumption on the simulation outputs, as this would admit the use of well-established tools associated with Brownian motion. While normality is justified by batching and the Central Limit Theorem (CLT), the assumption typically fails when simulations are run under an estimate of  $\theta^c$ , especially if such an estimate is updated in an online fashion. In this chapter, we build our algorithms on a Sequential Elimination framework [86, 87, 88], as it allows us to construct valid continuation regions even in the presence of IU. Here we use a production-inventory problem (see Section 4.4 for details) to illustrate how our algorithm works.

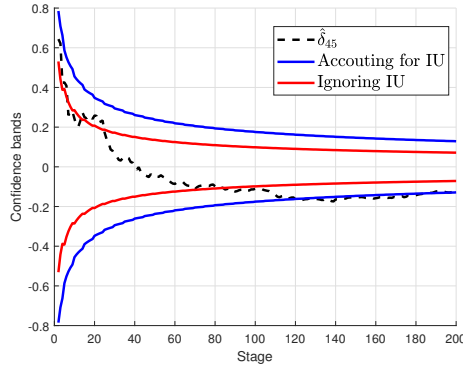


Figure 4.1: Continuation regions: accounting for IU and ignoring IU.

Figure 4.1 shows two continuation regions for comparing designs 4 and 5, where the area between the blue curves is the region constructed by our algorithm, and the area between the red curves is the region constructed by ignoring IU. The dashed line is the trajectory of  $\hat{\delta}_{45}$  across different stages. A continuation region works as follows. If  $\hat{\delta}_{45}$  exits

the region from above, then we conclude  $\delta_{45} > 0$  and vice versa. Notice that in the early stages, the estimate  $\hat{\delta}_{45}$  deviates from  $\delta_{45}(\theta^c) \approx -0.1$  due to IU and SU. If we use the continuation region constructed by ignoring IU, then we would mistakenly conclude that  $\delta_{45} > 0$ . In contrast, our algorithm accounts for IU by enlarging the continuation region, which ensures a correct comparison result with a desired probability.

The road map for the fixed confidence formulation is laid out as follows. First, we formulate the problem mathematically in Section 4.2.1. Then, we develop an algorithm, SE-IU, in Section 4.2.3 by directly extending the Sequential Elimination framework. In Section 4.2.4, we improve SE-IU by proposing a pairwise comparison algorithm. Theoretical guarantees are provided for both algorithms when using the true values of parameters. In addition, we propose a heuristic method to further boost selection efficiency in Section 4.2.5. Finally, Section 4.2.6 gives some guidance on implementation.

#### 4.2.1 Problem Setup

Suppose that new batches of i.i.d. input data arrive sequentially, and our goal is to continuously reduce IU and SU in order to identify the best design with high confidence. More specifically, we would like our R&S algorithm to run over a number of “stages”, where at each stage the following two steps are carried out.

- (i) For every input distribution  $P_{\theta^c(q)}$ ,  $1 \leq q \leq Q$ , collect  $k_q > 0$  additional new data samples to update the estimate of  $\theta^c(q)$ .
- (ii) For each design  $i \in \mathcal{I}$ , run additional  $R > 0$  replications under the new estimate of  $\theta^c$ , and update the estimate of  $H_i(\theta^c)$ .

For simplicity,  $k_q$  and  $R$  are assumed to be fixed constants across different stages. We call an algorithm *valid* if it selects the best design with a guaranteed PCS upon termination at a certain stage. The validness of an algorithm hinges on three aspects.

1. *Choice of estimator.* What estimator is used to estimate  $\theta^c$ ? The choice will affect

the properties of the online estimator of  $H_i(\theta^c)$ , as well as the difficulty of designing a continuation region.

2. *Online estimation.* Although the estimate of  $\theta^c$  gets increasingly accurate over the stages, the estimate of  $H_i(\theta^c)$  cannot converge to its true value without reusing the simulation outputs from previous stages. How should we approach this online estimation problem?
3. *Algorithm design.* The fixed confidence formulation essentially seeks to find a stopping time  $\tau^*$  such that by the  $\tau^*$ th stage, we can confidently determine which design is the best one. How can we design  $\tau^*$  to make  $\mathbb{E}[\tau^*]$  as small as possible?

Regarding the first aspect, we will restrict our discussion to a specific type of estimator. Let  $\hat{\theta}_{N_q}(q)$  be  $\theta^c(q)$ 's estimate using  $N_q$  data samples, and recall that  $\{\zeta_1(q), \dots, \zeta_{N_q}(q)\}$  are the input data. The following assumption is made to make the analysis more tractable.

**Assumption 4.2.1.** *For each input parameter  $\theta^c(q)$ , its estimator can be written in the form of  $\hat{\theta}_{N_q}(q) = \frac{1}{N_q} \sum_{j=1}^{N_q} G_q(\zeta_j(q))$ , where  $G_q : \mathbb{R}^{m_q} \rightarrow \mathbb{R}^{d_q}$  and  $\mathbb{E}[G_q(\zeta_1(q))] = \theta^c(q)$ .*

Assumption 4.2.1 can often be satisfied through reparametrization. For example, the normal distribution can be reparametrized by its first two moments, and then  $\hat{\theta}_{N_q}(q)$  corresponds to the moment estimators. Under Assumption 4.2.1, our problem setting can be simplified considerably. During the  $n$ th stage, we collect  $k_q$  additional data samples  $\{\zeta_j(q) \mid j = (n-1)k_q + 1, \dots, nk_q\}$  for the  $q$ th input model, and the sample mean of these incremental samples is

$$D_n(q) := \frac{1}{k_q} \sum_{j=(n-1)k_q+1}^{nk_q} G_q(\zeta_j(q)),$$

which can be viewed as a single batched data sample with variance shrunk by a factor of

$k_q$ . It can be easily checked that

$$\frac{1}{n} \sum_{j=1}^n D_j(q) = \frac{1}{nk_q} \sum_{j=1}^{nk_q} G_q(\zeta_j(q)), \quad \forall 1 \leq q \leq Q.$$

We may therefore gather these incremental estimates as  $D_n := [D_n(1)^\top, \dots, D_n(Q)^\top]^\top$ , a vector in  $\mathbb{R}^d$ . In other words, without loss of generality, we can assume that at the end of the  $n$ th stage, the estimator of  $\theta^c$  takes the form of  $\hat{\theta}_n = \frac{1}{n} \sum_{j=1}^n D_j$ , where  $D_j$  are i.i.d. samples with  $\mathbb{E}[D_1] = \theta^c$ . Similarly, it suffices to consider  $R = 1$ , i.e., when only one additional simulation replication is run at each stage. From this point on, our problem setting is simplified as follows. During the  $n$ th stage,

- (i) first collect one data sample  $D_n$ , and compute  $\hat{\theta}_n = \frac{n-1}{n} \hat{\theta}_{n-1} + \frac{1}{n} D_n$ ;
- (ii) then, for each design, run one more independent simulation replication under  $\hat{\theta}_n$ , and aggregate the simulation output with the previous ones.

#### 4.2.2 Moving Average Estimator

For the online estimation problem described in Section 4.2.1, a consistent estimator of  $H_i(\theta^c)$  can be constructed in various ways. For instance, simply averaging all the simulation outputs  $\{h_i(\xi_{in})\}_n$  usually ensures consistency. An alternative is to use a likelihood ratio estimator by reweighting the simulation outputs, but due to the correlation among  $\{\hat{\theta}_n\}$ , the resulting estimator will be biased (see [89] for insights into this observation).

Since our ultimate goal is to solve the R&S problem, the main challenge lies in finding an estimator which facilitates the design of a valid algorithm. Let  $\hat{H}_{i,n}$  denote the estimate of  $H_i(\theta^c)$  at the end of the  $n$ th stage. We construct an estimator by discarding the first (or the “oldest”)  $n_\eta := \lfloor \eta n \rfloor$ ,  $\eta \in (0, 1)$ , simulation outputs and then averaging the rest, i.e.,

$$\hat{H}_{i,n} := \frac{1}{n - n_\eta} \sum_{r=n_\eta+1}^n h_i(\xi_{ir}), \quad i \in \mathcal{I}. \quad (4.2.1)$$

The estimator in (4.2.1) will be referred to as a *moving average estimator*, since it averages simulation outputs within a moving and expanding time window. The motivation is to throw away some of those “outdated” simulation outputs which were generated under less accurate estimates of  $\theta^c$ . We establish the asymptotic normality of  $\hat{H}_{i,n}$  in the following theorem.

**Theorem 4.2.1.** *Let Assumption 4.2.1 hold. Further suppose that  $\Sigma_G := \text{Cov}[D_1]$  exists and  $H_i$  is twice continuously differentiable at  $\theta^c$ . Then, for any  $\eta \in [0, 1)$ ,*

$$\sqrt{n}[\hat{H}_{i,n} - H_i(\theta^c)] \Rightarrow \mathcal{N}(0, \tilde{\sigma}_{i,\infty}^2) \quad \text{as } n \rightarrow \infty,$$

where

$$\tilde{\sigma}_{i,\infty}^2 := w_\eta \nabla H_i(\theta^c)^\top \Sigma_G \nabla H_i(\theta^c) + \frac{1}{1-\eta} \sigma_i^2(\theta^c),$$

with  $\nabla$  being the gradient, and

$$w_\eta := \frac{2}{1-\eta} + \frac{2\eta \log \eta}{(1-\eta)^2}.$$

Before presenting the proof, we note that Theorem 4.2.1 is an interesting result in its own right. It shows that the limiting variance  $\tilde{\sigma}_{i,\infty}^2$  is again a weighted sum of variances caused by IU and SU, which are  $\tilde{V}_I := \nabla H_i(\theta^c)^\top \Sigma_G \nabla H_i(\theta^c)$  and  $\tilde{V}_S := \sigma_i^2(\theta^c)$ , respectively. To interpret the weights, we look at the following cases.

- (i) Setting  $\eta = 0$  gives  $w_\eta = 2$ , meaning that if we retain all the outputs, then the variance caused by IU, corresponding to  $\tilde{V}_I$ , will be doubled.
- (ii) Sending  $\eta \rightarrow 1$  gives  $w_\eta \rightarrow 1$ . This loosely corresponds to the case of  $\hat{H}_{i,n} = h_i(\xi_{in})$ , where we only retain the single most recent output. As a result,  $\hat{H}_{i,n}$  is free from the error accumulated over previous estimates of  $\theta^c$ , and thus  $\tilde{V}_I$  is not inflated. However,  $\tilde{V}_S$  is inflated by a factor  $1/(1-\eta) \rightarrow \infty$ , since the effective number of outputs is not tending to  $\infty$  as  $n \rightarrow \infty$ .



(iii) A balance between IU and SU can be achieved by choosing the  $\eta$  that minimizes

$$\tilde{\sigma}_{i,\infty}^2.$$

Roughly speaking, the parameter  $\eta$  captures a bias-variance tradeoff. On the one hand, discarding previous outputs helps reduce the bias  $H_i(\hat{\theta}_n) - H_i(\theta^c)$  due to IU. On the other hand, the variance caused by SU gets inflated if we average fewer simulation outputs. In Section 4.2.3, we will explain the role of moving average estimator in designing a valid algorithm. At this point, an important note is that *simply ignoring IU and applying existing algorithms may result in undershooting the PCS target*. For example, in the production-inventory problem to be considered in Section 4.4, if we apply a traditional Sequential Elimination algorithm for  $k_q = R = 100$  with a target PCS of 95%, then the resulting PCS will only be around 86%.

The following lemmas will be useful for proving Theorem 4.2.1.

**Lemma 4.2.1** (The Lindeberg-Feller Theorem (see, e.g., Theorem 3.4.5 [63])). *For each  $n$ , let  $Y_{n,i}$ ,  $1 \leq i \leq n$  be independent r.v.s with  $EY_{n,i} = 0$ . Suppose*

$$(i) \sum_{i=1}^n \mathbb{E}Y_{n,i}^2 \rightarrow \sigma^2 > 0.$$

$$(ii) \text{ For all } \epsilon > 0, \lim_{n \rightarrow \infty} \sum_{i=1}^n \mathbb{E}[|Y_{n,i}|^2 \mathbb{1}_{\{|Y_{n,i}| > \epsilon\}}] = 0.$$

*Then  $\sum_{i=1}^n Y_{n,i} \Rightarrow \mathcal{N}(0, \sigma^2)$  as  $n \rightarrow \infty$ .*

**Lemma 4.2.2.** *Let  $\{X_n\}$  be independent r.v.s with  $\mathbb{E}X_n = 0$ . If  $X_n \Rightarrow X$  and  $\mathbb{E}X_n^2 \rightarrow \mathbb{E}X^2$  as  $n \rightarrow \infty$ , then for any  $\eta \in (0, 1)$ ,*

$$\frac{1}{\sqrt{n - n_\eta}} \sum_{i=n_\eta+1}^n X_i \Rightarrow \mathcal{N}(0, \mathbb{E}X^2) \quad \text{as } n \rightarrow \infty.$$

*Proof of Lemma 4.2.2.* Let  $Y_{n,i} := 0$  if  $i \leq n_\eta$  and  $X_i/\sqrt{n - n_\eta}$  otherwise. We will apply Lemma 4.2.1 to  $Y_{n,i}$ . Condition (i) is satisfied since

$$\sum_{i=1}^n \mathbb{E}Y_{n,i}^2 = \sum_{i=n_\eta+1}^n \mathbb{E}X_i^2/(n - n_\eta) \rightarrow \mathbb{E}X^2.$$

In addition,  $X_n \Rightarrow X$  implies that there exists  $\tilde{X}_n \stackrel{\mathcal{D}}{=} X_n$ ,  $\tilde{X} \stackrel{\mathcal{D}}{=} X$  such that  $\tilde{X}_n \rightarrow \tilde{X}$  almost surely (a.s.) as  $n \rightarrow \infty$ . Since  $\{\tilde{X}_n\}$  is a.s. finite,

$$\mathbb{E} \left[ |X_n|^2 \mathbb{1}_{\{|X_n| > \epsilon \sqrt{n-n_\eta}\}} \right] = \mathbb{E} \left[ |\tilde{X}_n|^2 \mathbb{1}_{\{|\tilde{X}_n| > \epsilon \sqrt{n-n_\eta}\}} \right] \rightarrow 0$$

by a generalized Dominated Convergence Theorem (note that the integrand is dominated by  $|\tilde{X}_n|^2$  and  $\mathbb{E}\tilde{X}_n \rightarrow \mathbb{E}\tilde{X}$ ). Thus, as  $n \rightarrow \infty$ ,

$$\sum_{i=1}^n \mathbb{E}[|Y_{n,i}|^2 \mathbb{1}_{\{|Y_{n,i}| > \epsilon\}}] = \frac{1}{n - n_\eta} \sum_{i=n_\eta+1}^n \mathbb{E}[|X_i|^2 \mathbb{1}_{\{|X_i| > \epsilon \sqrt{n-n_\eta}\}}] \rightarrow 0,$$

which verifies condition (ii), and the result follows.  $\square$

**Lemma 4.2.3.** *Let  $\gamma_{n,i} := \sum_{j=i}^n \frac{1}{j}$  and  $a_k := \sum_{i=1}^k \gamma_{n,i}^2$ . Then, for all  $k \leq n-1$ ,*

$$a_k = k - \gamma_{k,1} + k(1 + \gamma_{k+1,n})^2,$$

and for  $k = n$ ,  $a_n = 2n - \gamma_{n,1}$ .

*Proof of Lemma 4.2.3.* For  $k \leq n-1$ , we have by induction

$$\begin{aligned} a_k &= (1 + \gamma_{n,2})^2 + \gamma_{n,2}^2 + \gamma_{n,3}^2 + \cdots + \gamma_{n,k}^2 \\ &= 1 + 2\gamma_{n,2} + 2\gamma_{n,2}^2 + \gamma_{n,3}^2 + \cdots + \gamma_{n,k}^2 \\ &= 1 + 2\gamma_{n,2} + 2\left(\frac{1}{2} + \gamma_{n,3}\right)^2 + \gamma_{n,3}^2 + \cdots + \gamma_{n,k}^2 \\ &= 1 + \frac{1}{2} + 2(\gamma_{n,2} + \gamma_{n,3}) + 3\gamma_{n,3}^2 + \cdots + \gamma_{n,k}^2 \\ &\quad \vdots \\ &= \gamma_{k-1,1} + 2 \sum_{i=2}^k \gamma_{n,i} + k\gamma_{n,k}^2, \end{aligned}$$

where note that

$$\begin{aligned}
\sum_{i=2}^k \gamma_{n,i} &= \sum_{i=2}^k \sum_{j=i}^n \frac{1}{j} = \sum_{j=2}^k \sum_{i=2}^j \frac{1}{j} + (k-1) \sum_{j=k+1}^n \frac{1}{j} \\
&= \sum_{j=2}^k \frac{j-1}{j} + (k-1) \sum_{j=k+1}^n \frac{1}{j} \\
&= (k-1) - \sum_{j=2}^k \frac{1}{j} + (k-1) \sum_{j=k+1}^n \frac{1}{j}.
\end{aligned}$$

The result is clear from a direct computation, and the case of  $k = n$  follows similarly.  $\square$

*Proof of Theorem 4.2.1.* For simplicity, we suppress the subscript  $i$  and replace the scaling factor  $\sqrt{n}$  with  $\sqrt{n - n_\eta}$ .

$$\begin{aligned}
&\sqrt{n - n_\eta} \left( \frac{1}{n - n_\eta} \sum_{j=n_\eta+1}^n h(\xi_j) - H(\theta^c) \right) \\
&= \underbrace{\frac{1}{\sqrt{n - n_\eta}} \sum_{j=n_\eta+1}^n [h(\xi_j) - H(\hat{\theta}_j)]}_{X_n} + \underbrace{\frac{1}{\sqrt{n - n_\eta}} \sum_{j=n_\eta+1}^n [H(\hat{\theta}_j) - H(\theta^c)]}_{Y_n}.
\end{aligned}$$

Let  $\mathcal{F}_n := \sigma(D_1, \dots, D_n)$ . The characteristic function of  $X_n + Y_n$  is

$$\mathbb{E}[e^{it(X_n + Y_n)}] = \mathbb{E} \left\{ e^{itY_n} \mathbb{E}[e^{itX_n} \mid \mathcal{F}_n] \right\}.$$

Note that conditioned on  $\mathcal{F}_n$ ,  $h(\xi_j) - H(\hat{\theta}_j)$  are independent r.v.s with mean 0 and variance  $\sigma^2(\hat{\theta}_j)$ . Since  $\hat{\theta}_n \rightarrow \theta^c$  a.s. by the Strong Law of Large Numbers,  $\sigma^2(\hat{\theta}_n) \rightarrow \sigma^2(\theta^c)$ , and Lemma 4.2.2 implies that  $\mathbb{E}[e^{itX_n} \mid \mathcal{F}_n] \rightarrow \exp(-\sigma^2(\theta^c)t^2/2)$  a.s. On the other hand, apply a Taylor expansion to  $Y_n$  around  $\theta^c$  and we have

$$Y_n = \frac{\nabla H(\theta^c)^\top}{\sqrt{n - n_\eta}} \sum_{i=n_\eta+1}^n (\hat{\theta}_i - \theta^c) + \frac{1}{\sqrt{n - n_\eta}} \sum_{i=n_\eta+1}^n (\hat{\theta}_i - \theta^c)^\top \nabla^2 H(\tilde{\theta}_i) (\hat{\theta}_i - \theta^c), \quad (4.2.2)$$

where  $\tilde{\theta}_i = \lambda \hat{\theta}_i + (1 - \lambda)\theta^c$  for some  $\lambda \in [0, 1]$ . For the first term in the RHS of (4.2.2), we focus on the case of  $\theta^c \in \mathbb{R}$  since it can be easily extended to  $\mathbb{R}^d$  via the Cramér-Wold device (see Theorem 3.9.5 in [63]). We will apply Lemma 4.2.1 to the second term. By assumption  $\hat{\theta}_n = \sum_{i=1}^n D_i/n$ , thus

$$\begin{aligned} \frac{1}{\sqrt{n - n_\eta}} \sum_{i=n_\eta+1}^n (\hat{\theta}_i - \theta^c) &= \frac{1}{\sqrt{n - n_\eta}} \sum_{i=n_\eta+1}^n \frac{1}{i} \sum_{j=1}^i (D_j - \theta^c) \\ &= \frac{1}{\sqrt{n - n_\eta}} \sum_{i=n_\eta+1}^n \gamma_{n,i} (D_i - \theta^c), \end{aligned}$$

where  $\gamma_{n,i} := \sum_{j=i}^n \frac{1}{j}$ . Noting that  $(D_i - \theta^c)$  are i.i.d. r.v.s with mean 0 and variance  $\Sigma_G$ ,

$$\frac{\sum_{i=n_\eta+1}^n \gamma_{n,i}^2}{n - n_\eta} \mathbb{E}[|D_1 - \theta^c|^2] \rightarrow (1 - \eta)w_\eta \Sigma_G \quad \text{as } n \rightarrow \infty,$$

where the factor  $(1 - \eta)w_\eta$  is a consequence of Lemma 4.2.3. Furthermore, it follows from  $\gamma_{n,1} \sim \log n$  that  $\sqrt{n - n_\eta}/\gamma_{n,1} \rightarrow \infty$  as  $n \rightarrow \infty$ . Therefore, for any  $\epsilon > 0$ ,

$$\begin{aligned} &\sum_{i=n_\eta+1}^n \mathbb{E} \left[ \frac{\gamma_{n,i}^2}{n - n_\eta} (D_i - \theta^c)^2 \mathbb{1}_{\{\gamma_{n,i}|D_i - \theta^c| > \epsilon \sqrt{n - n_\eta}\}} \right] \\ &\leq \frac{\sum_{i=n_\eta+1}^n \gamma_{n,i}^2}{n - n_\eta} \mathbb{E} \left[ (D_1 - \theta^c)^2 \mathbb{1}_{\{|D_1 - \theta^c| > \epsilon \sqrt{n - n_\eta}/\gamma_{n,1}\}} \right] \rightarrow 0 \end{aligned}$$

by the Dominated Convergence Theorem, and Lemma 4.2.1 implies that

$$\frac{1}{\sqrt{n - n_\eta}} \sum_{i=n_\eta+1}^n (\hat{\theta}_i - \theta^c) \Rightarrow \mathcal{N}(0, (1 - \eta)w_\eta \Sigma_G).$$

It remains to show that the last term in (4.2.2) vanishes. Let  $\lambda_i(A)$  denote the  $i$ th largest eigenvalue of a matrix  $A$  and define  $\lambda^*(A) = \max_i |\lambda_i(A)|$ . It follows from the continuity of  $\nabla^2 H(\cdot)$  that  $\lambda^*(\nabla^2 H(\tilde{\theta}_n)) \rightarrow \lambda^*(\nabla^2 H(\theta^c))$  a.s. as  $n \rightarrow \infty$ , so there exists a.s.  $M_1 > 0$  such that  $\lambda^*(\nabla^2 H(\tilde{\theta}_n)) < M_1$  for all  $n$ . Also, by the Law of the Iterated Logarithm (see,

e.g., [63]), there exists a.s.  $M_2 > 0$  such that

$$\|\hat{\theta}_n - \theta^c\| \leq \frac{1}{n} \sum_{j=1}^d \left| \sum_{i=1}^n (D_{ij} - \theta_j^c) \right| \leq M_2 \sqrt{\frac{\log \log n}{n}}, \quad \forall n \geq 3,$$

where  $D_{ij}$  and  $\theta_j^c$  denote the  $j$ th coordinate of  $D_i$  and  $\theta^c$ , respectively. Combining these two bounds and by increasing  $M_2$  if necessary, we have for all  $n$  large enough,

$$\begin{aligned} & \frac{1}{\sqrt{n - n_\eta}} \left| \sum_{i=n_\eta+1}^n (\hat{\theta}_i - \theta^c)^\top \nabla^2 H(\tilde{\theta}_i) (\hat{\theta}_i - \theta^c) \right| \\ & \leq \frac{1}{\sqrt{n - n_\eta}} \sum_{i=n_\eta+1}^n \lambda^*(\nabla^2 H(\tilde{\theta}_i)) \|\hat{\theta}_i - \theta^c\|^2 \\ & \leq \frac{M_1 M_2^2}{\sqrt{n - n_\eta}} \sum_{i=3}^n \frac{\log \log i}{i} \leq M_1 M_2^2 \frac{\log \log n}{\sqrt{n - n_\eta}} \sum_{i=3}^n \frac{1}{i} \leq M_1 M_2^2 \frac{(\log n)^2}{\sqrt{n - n_\eta}}, \end{aligned}$$

which converges to 0 as  $n \rightarrow \infty$ . Following the argument in the proof of Theorem 4.3.1 for the characteristic function of  $X_n + Y_n$ , we have

$$\sqrt{n - n_\eta} [\hat{H}_{i,n} - H_i(\theta^c)] \Rightarrow \mathcal{N}(0, (1 - \eta) \sigma_{i,\infty}^2), \quad \text{as } n \rightarrow \infty.$$

Finally, rescaling the limiting variance by a factor of  $(1 - \eta)^{-1}$  concludes the proof.  $\square$

#### 4.2.3 The SE-IU Algorithm

Our first algorithm is a direct extension of a Sequential Elimination framework proposed by Even-Dar et al. [86, 87], which was also discussed in [88] recently. This general paradigm has a simple structure and can be extended to handle IU. Given  $\alpha \in (0, 1)$ , the idea is to construct confidence bounds  $\{c_{i,n}\}$  on  $\hat{H}_{i,n}$  for each design  $i$  such that

$$\mathbb{P}\{|\hat{H}_{i,n} - H_i(\theta^c)| \leq c_{i,n}, \forall i, n\} \geq 1 - \alpha, \quad \alpha \in (0, 1), \quad (4.2.3)$$

where  $c_{i,n} \rightarrow 0$  as  $n \rightarrow \infty$ . At each stage  $n$ , a design  $i$  gets eliminated if

$$\hat{H}_{i,n} + c_{i,n} < \max_{j \neq i} \left\{ \hat{H}_{j,n} - c_{j,n} \right\}.$$

In other words, a design is eliminated if its upper confidence bound is below some other design's lower confidence bound. Then, on the event  $\mathcal{E} := \left\{ |\hat{H}_{i,n} - H_i(\theta^c)| \leq c_{i,n}, \forall i, n \right\}$ , we have for any  $i \neq b$ ,

$$\hat{H}_{b,n} + c_{b,n} - (\hat{H}_{i,n} - c_{i,n}) \geq \delta_{bi}(\theta^c) > 0, \quad \forall n.$$

Therefore, design  $b$  will never be eliminated on event  $\mathcal{E}$ . Since  $c_{i,n} \rightarrow 0$ , the algorithm terminates almost surely, and  $b$  will survive all eliminations with probability at least  $1 - \alpha$ . By (4.2.3), this delivers the desired PCS guarantee.

The key to efficiently ruling out inferior designs is to find tight confidence bounds  $\{c_{i,n}\}$  that satisfy (4.2.3). When there is no IU, this can be easily done using well-known concentration inequalities on  $\hat{H}_i(\theta^c)$ , such as the Chernoff bound and Hoeffding's inequality. In the presence of IU, these inequalities do not apply directly and a new concentration bound needs to be derived for  $\hat{H}_{i,n}$ . The following assumption will be useful to this end.

**Assumption 4.2.2.**

- (i) For all  $1 \leq j \leq d$ , the  $j$ th coordinate of  $D_n$  is sub-Gaussian with parameter  $\nu_j$ .
- (ii) For any  $\theta \in \Theta$ , if  $\xi \sim P_\theta$ , then  $h_i(\xi)$  is sub-Gaussian.
- (iii) For all  $u > 0$  and any design  $i$ , there exists a function  $L_i(\cdot) > 0$  such that

$$|H_i(\theta_1) - H_i(\theta_2)| \leq L_i(u) \|\theta_1 - \theta_2\|, \quad \forall \theta_1, \theta_2 \in \{\theta \in \Theta \mid \|\theta - \theta^c\| \leq u\}.$$

- (iv) For any design  $i$ ,  $\sigma_i^2(\cdot)$  is a continuous function.

Assumption 4.2.2 (i) and (ii) may appear restrictive at first sight. For example, the input distributions in an M/M/1 queue simulation model are sub-exponential but not sub-Gaussian. However, we make these assumptions mainly to avoid unnecessary technicality, and we will show numerically that our algorithm works even if these conditions are not met.

To get a sense of how to meet the guarantee in (4.2.3), consider constructing confidence bounds  $c_{i,n}$  such that

$$\mathbb{P} \left\{ \{ |\hat{H}_{i,n} - H_i(\theta^c)| \leq c_{i,n}, \forall n \}^c \right\} \leq \beta \quad (4.2.4)$$

for some  $\beta \in (0, 1)$ , where “c” denotes complement. One way is to consider an event

$$A_u := \{ \|\hat{\theta}_n - \theta^c\| \leq u, \forall n \}$$

for some  $u > 0$ . Then, the guarantee in (4.2.4) can be met if we can control

$$\mathbb{P} \left\{ A_u \cap \{ |\hat{H}_{i,n} - H_i(\theta^c)| \leq c_{i,n}, \forall n \}^c \right\} + \mathbb{P}(A_u^c), \quad (4.2.5)$$

since it is an upper bound on the left-hand side (LHS) in (4.2.4). Note that  $\mathbb{P}(A_u^c)$  can be controlled by enlarging  $u$ . Meanwhile, on the event  $A_u$ , we have  $H_i$  being Lipschitz continuous and  $\sigma_i(\hat{\theta}_n)$  being bounded, where it is possible to derive a concentration bound for  $|\hat{H}_{i,n} - H_i(\theta^c)|$  through a decomposition,

$$|\hat{H}_{i,n} - H_i(\theta^c)| \leq |\hat{H}_{i,n} - H_i(\hat{\theta}_n)| + |H_i(\hat{\theta}_n) - H_i(\theta^c)|.$$

The rest is to combine all the bounds through a union bound, where the choice of the estimator  $\hat{H}_{i,n}$  is crucial. For example, if we simply average all the simulation outputs, then the bound will be infinite due to cumulative bias. Using the moving average estimator,

however, we are able to construct  $c_{i,n}$  that satisfies (4.2.4) by virtue of a bias-variance tradeoff (as long as  $\eta > 0$ ).

The upcoming SE-IU algorithm relies on some key parameters including  $\{\nu_j\}$ ,  $\{\sigma_i\}$  and  $\{L_i\}$ . For now, we present an ideal version of the algorithm by assuming full knowledge of these parameters, and defer implementation details to Section 4.2.6.

*Algorithm: SE-IU (ideal version)*

- **Input.**  $\alpha \in (0, 1), \eta \in (0, 1), K \geq 2, n_0 \geq 10$ .
- **Step 1.** Solve the following equation in  $u$ , and let  $u^*$  be the solution.

$$\sum_{j=1}^d \frac{\exp\left(-\frac{(n_0+1)u^2}{2d\nu_j^2}\right)}{1 - \exp\left(-\frac{u^2}{2d\nu_j^2}\right)} = \frac{\alpha}{6}. \quad (4.2.6)$$

- **Step 2.** For each design, compute

$$\bar{\sigma}_i := \sup_{\substack{\|\theta - \theta^c\| \leq u^* \\ \theta \in \Theta}} \sigma_i(\theta), \quad \bar{L}_i := L_i(u^*),$$

as well as the constants

$$\kappa_{n_0} := \sum_{n=n_0+1}^{\infty} n^{-2}, \quad \beta_{n_0} := \sum_{n=n_0+1}^{\infty} (n - n_\eta)^{-2}.$$

Let  $\bar{\nu} := \max_j \nu_j$ . Run  $n_0$  stages and set  $n \leftarrow n_0 + 1$ . Also set  $\mathcal{S} \leftarrow \{1, 2, \dots, K\}$ .

- **Step 3.** Run an additional stage for all designs  $1, 2, \dots, K$ , and compute their estimates  $\hat{H}_{i,n}$  using the moving average estimator in (4.2.1).
- **Step 4.** Compute the confidence bounds  $c_{i,n}$  for each design  $i$ , where  $c_{i,n} = t_{i,n} + r_{i,n}$



and

$$t_{i,n} := 2\bar{\sigma}_i \sqrt{\frac{\ln \left( \sqrt{\frac{6K\kappa_{n_0}}{\alpha}} n \right)}{n - n_\eta}}, \quad r_{i,n} := \bar{\nu} \bar{L}_i \sqrt{\frac{6d \ln \left( \left( \frac{6dK\beta_{n_0}}{\alpha} \right)^{\frac{1}{3}} (n - n_\eta) \right)}{n_\eta + 1}}. \quad (4.2.7)$$

For each  $i \in \mathcal{S}$ , if

$$\hat{H}_{i,n} + c_{i,n} < \max_{j \neq i} \left( \hat{H}_{j,n} - c_{j,n} \right),$$

then set  $\mathcal{S} \leftarrow \mathcal{S} \setminus \{i\}$ . Go to Output if  $|\mathcal{S}| = 1$ ; otherwise, set  $n \leftarrow n + 1$  and go to Step 3.

- **Output.** Select the only design in  $\mathcal{S}$  as the best one.

Some important features of SE-IU are outlined as follows.

1. First, the width of  $\{c_{i,n}\}$  are of order  $O(\sqrt{\ln(n)/n})$ , which is standard for sequential elimination algorithms. However, the confidence bounds are widened, where  $t_{i,n}$  and  $r_{i,n}$  correspond to SU and IU, respectively.
2. Second, we do not eliminate any design in the first  $n_0$  stages. In view of (4.2.6), a larger  $n_0$  leads to a smaller  $u^*$ , which in turn gives us smaller  $\bar{\sigma}_i, \bar{L}_i, \kappa_{n_0}$  and  $\beta_{n_0}$ , hence tighter confidence bounds. Also, equation (4.2.6) always has a unique solution, since the LHS is a continuous and monotone function of  $u$  with range  $(0, \infty)$ .
3. Third, the running time of SE-IU primarily depends on the parameters  $\nu_j, \bar{\sigma}_i, \bar{L}_i$ , and  $\delta_{bi}(\theta^c)$ . For instance, if  $\bar{\sigma}_i$  is increased by a factor of  $k > 1$ , then it would take at least  $k^2$  times as many stages to reach the same width of confidence bounds.

Let  $\tau^*$  be the number of stages until the algorithm terminates. A nice property of the Sequential Elimination framework is that it is automatically equipped with an upper bound on  $\mathbb{E}[\tau^*]$ .

**Theorem 4.2.2.** *Let Assumption 4.2.2 hold. Then, the SE-IU algorithm guarantees to select the best design with probability at least  $1 - \alpha$ . Furthermore,*

$$\mathbb{E}[\tau^*] \leq 2 \sum_{i \neq b} \tau_i^* + 4(K-1)(\alpha + 2de^{-\mathcal{K}}(1 - e^{-\mathcal{K}})^{-2}),$$

where  $\tau_i^* := \inf\{n > n_0 \mid 2(c_{b,n} + c_{i,n}) \leq \delta_{bi}(\theta^c)\}$  and  $\mathcal{K} := \eta(u^*)^2/(2d\bar{\nu}^2)$ .

The dominating term in Theorem 4.2.2's bound is  $\sum_{i \neq b} \tau_i^*$ , where each  $\tau_i^*$  characterizes the difficulty in eliminating design  $i$ . For example, if design  $i$  has a large variance  $\sigma_i^2(\theta^c)$  and a small gap  $\delta_{bi}(\theta^c)$ , then  $\tau_i^*$  would be large, and it will take longer to eliminate design  $i$ . Given the same performance gap  $\delta_{bi}(\theta^c)$ ,  $\tau_i^*$  primarily depends on  $\{c_{i,n}\}$ , i.e., the width of the confidence bounds. In Sections 4.2.4 and 4.2.5, we discuss how to tighten the confidence bounds in order to achieve faster stopping.

*Proof of Theorem 4.2.2.* First, we show the validity of SE-IU. According to our discussion in Section 4.2.3, it suffices to show that  $\mathbb{P}(\mathcal{E}_{n_0}^c) \leq \alpha$ , where

$$\mathcal{E}_{n_0} := \left\{ |\hat{H}_{i,n} - H_i(\theta^c)| \leq c_{i,n}, \forall i, n \geq n_0 + 1 \right\}.$$

Letting  $A_{u^*} := \bigcap_{n=n_0+1}^{\infty} \{\|\hat{\theta}_n - \theta^c\| \leq u^*\}$ , we have the following upper bound,

$$\mathbb{P}(\mathcal{E}_{n_0}^c) \leq \mathbb{P}(\mathcal{E}_{n_0}^c \cap A_{u^*}) + \mathbb{P}(A_{u^*}^c).$$

Furthermore, let  $\bar{H}_{i,n} := \frac{1}{n-n_\eta} \sum_{j=n_\eta+1}^n H_i(\hat{\theta}_j)$  and we have

$$\begin{aligned} \mathbb{P}(\mathcal{E}_{n_0}^c) &\leq \sum_{i=1}^K \sum_{n=n_0+1}^{\infty} \mathbb{P} \left\{ \{|\hat{H}_{i,n} - \bar{H}_{i,n}| > t_{i,n}\} \cup \{|\bar{H}_{i,n} - H_i(\theta^c)| > r_{i,n}\} \cap A_{u^*} \right\} \\ &\quad + \mathbb{P}(A_{u^*}^c). \end{aligned}$$

In particular, due to Assumption 4.2.2 (iii),

$$\begin{aligned} \{|\bar{H}_{i,n} - H_i(\theta^c)| > r_{i,n}\} \cap A_{u^*} &= \left\{ \left| \sum_{j=n_\eta+1}^n [H_i(\hat{\theta}_j) - H_i(\theta^c)] \right| > (n - n_\eta)r_{i,n} \right\} \cap A_{u^*} \\ &\subseteq \bigcup_{j=n_\eta+1}^n \left\{ \|\hat{\theta}_j - \theta^c\| > r_{i,n}/\bar{L}_i \right\} \cap A_{u^*}. \end{aligned}$$

Putting all these together, we have

$$\begin{aligned} \mathbb{P}(\mathcal{E}_{n_0}^c) &\leq \sum_{i=1}^K \sum_{n=n_0+1}^{\infty} \mathbb{P} \left\{ \{|\hat{H}_{i,n} - \bar{H}_{i,n}| > t_{i,n}\} \cap A_{u^*} \right\} \\ &\quad + \sum_{i=1}^K \sum_{n=n_0+1}^{\infty} \sum_{j=n_\eta+1}^n \mathbb{P} \left\{ \|\hat{\theta}_j - \theta^c\| > r_{i,n}/\bar{L}_i \right\} + \mathbb{P}(A_{u^*}^c). \end{aligned}$$

We will bound each term in this upper bound.

(i) By applying a sub-Gaussian tail bound to each dimension of  $(\hat{\theta}_n - \theta^c)$ ,

$$\begin{aligned} \mathbb{P}(A_{u^*}^c) &\leq \sum_{n=n_0+1}^{\infty} \mathbb{P} \left\{ \|\hat{\theta}_n - \theta^c\| > u^* \right\} \\ &\leq \sum_{n=n_0+1}^{\infty} \sum_{j=1}^d \mathbb{P} \left\{ |\hat{\theta}_{n,j} - \theta_j^c| > u^*/\sqrt{d} \right\} \\ &\leq 2 \sum_{n=n_0+1}^{\infty} \sum_{j=1}^d \exp \left( -\frac{n(u^*)^2}{2d\nu_j^2} \right) \\ &= 2 \sum_{j=1}^d \frac{\exp \left( -\frac{(n_0+1)(u^*)^2}{2d\nu_j^2} \right)}{1 - \exp \left( -\frac{(u^*)^2}{2d\nu_j^2} \right)} = \frac{\alpha}{3}, \end{aligned}$$

where the last equality follows from the definition of  $u^*$ .

(ii) Let  $\mathcal{F}_n := \sigma\{D_1, \dots, D_n\}$  and  $\mathcal{F}_\infty := \sigma(\cup_{n=1}^\infty \sigma(\mathcal{F}_n))$ . We have

$$\begin{aligned}
& \sum_{n=n_0+1}^\infty \mathbb{P} \left\{ \{|\hat{H}_{i,n} - \bar{H}_{i,n}| > t_{i,n}\} \cap A_{u^*} \right\} \\
&= \sum_{n=n_0+1}^\infty \mathbb{E} \left\{ \mathbb{P} \left\{ \{|\hat{H}_{i,n} - \bar{H}_{i,n}| > t_{i,n}\} \cap A_{u^*} \middle| \mathcal{F}_\infty \right\} \right\} \\
&\leq \sum_{n=n_0+1}^\infty \mathbb{E} \left\{ \mathbb{P} \left\{ \left| \frac{1}{n - n_\eta} \sum_{j=n_\eta+1}^n [h_i(\xi_{ij}) - H_i(\hat{\theta}_j)] \right| > t_{i,n} \middle| \mathcal{F}_\infty \right\} \mathbb{1}_{A_{u^*}} \right\} \\
&\leq \sum_{n=n_0+1}^\infty 2 \exp \left( -\frac{(n - n_\eta)t_{i,n}^2}{2\bar{\sigma}_i^2} \right) = \frac{\alpha}{3K},
\end{aligned}$$

where the last equality follows from the definition of  $t_{i,n}$ .

(iii) Again, using a sub-Gaussian bound on each dimension of  $(\hat{\theta}_j - \theta^c)$ ,

$$\begin{aligned}
& \sum_{n=n_0+1}^\infty \sum_{j=n_\eta+1}^n \mathbb{P} \left\{ \|\hat{\theta}_j - \theta^c\| > r_{i,n}/\bar{L}_i \right\} \\
&\leq \sum_{n=n_0+1}^\infty \sum_{j=n_\eta+1}^n 2d \exp \left( -\frac{j r_{i,n}^2}{2d\bar{L}_i^2 \bar{\nu}^2} \right) \\
&\leq \sum_{n=n_0+1}^\infty 2d(n - n_\eta) \exp \left( -\frac{(n_\eta + 1)r_{i,n}^2}{2d\bar{L}_i^2 \bar{\nu}^2} \right) = \frac{\alpha}{3K},
\end{aligned}$$

where the last inequality follows from the definition of  $r_{i,n}$ .

Gather all the inequalities and we have  $\mathbb{P}(\mathcal{E}_{n_0}^c) \leq \frac{\alpha}{3} + K \frac{\alpha}{3K} + K \frac{\alpha}{3K} = \alpha$ , thus proving the validity of SE-IU. Next, we prove the upper bound on  $\mathbb{E}[\tau^*]$ . Let  $n_i$  be the number of stages design  $i$  is in the set  $\mathcal{S}$ . If we can show that

$$\mathbb{E}[n_i] \leq \tau_i^* + 2(\alpha + 2de^{-\mathcal{K}}(1 - e^{-\mathcal{K}})^{-2}), \quad \forall i \neq b, \quad (4.2.8)$$

then the upper bound on  $\mathbb{E}[\tau^*]$  follows from  $\mathbb{E}[\tau^*] \leq 2 \sum_{i \neq b} \mathbb{E}[n_i]$ . To show (4.2.8), let

$$S_{i,n} := \{i \in \mathcal{S} \text{ at the } n\text{th stage}\}.$$

By the definition of  $\tau_i^*$ , we have  $c_{b,n} + c_{i,n} < \delta_{bi}(\theta^c)/2$  and  $S_{i,n} \subseteq \{\hat{H}_{b,n} - \hat{H}_{i,n} < c_{b,n} + c_{i,n}\}$  for all  $n > \tau_i^*$ . It follows that

$$\begin{aligned}
\mathbb{E}[n_i] &= \sum_{n=1}^{\tau_i^*} \mathbb{P}(S_{i,n}) + \sum_{n=\tau_i^*+1}^{\infty} \mathbb{P}(S_{i,n}) \\
&\leq \tau_i^* + \sum_{n=\tau_i^*+1}^{\infty} \mathbb{P}\left\{\hat{H}_{b,n} - \hat{H}_{i,n} < c_{b,n} + c_{i,n}\right\} \\
&\leq \tau_i^* + \sum_{n=\tau_i^*+1}^{\infty} \mathbb{P}\left\{\hat{H}_{b,n} - \hat{H}_{i,n} - (H_b(\theta^c) - H_i(\theta^c)) < -\delta_{bi}(\theta^c)/2\right\} \\
&\leq \tau_i^* + \sum_{n=\tau_i^*+1}^{\infty} \mathbb{P}\left\{\hat{H}_{b,n} - \hat{H}_{i,n} - (H_b(\theta^c) - H_i(\theta^c)) < -(c_{b,n} + c_{i,n})\right\} \\
&\leq \tau_i^* + \sum_{n=\tau_i^*+1}^{\infty} \mathbb{P}\{\hat{H}_{b,n} - H_b(\theta^c) < -c_{b,n}\} + \sum_{n=\tau_i^*+1}^{\infty} \mathbb{P}\{\hat{H}_{i,n} - H_i(\theta^c) > c_{i,n}\}.
\end{aligned}$$

We bound the first sum in the last inequality, since the other can be bounded similarly.

Consider

$$B_n := \bigcap_{\ell=n_\eta+1}^n \{\|\hat{\theta}_\ell - \theta^c\| \leq u^*\}.$$

Then, we have

$$\begin{aligned}
&\sum_{n=\tau_i^*+1}^{\infty} \mathbb{P}\{\hat{H}_{b,n} - H_b(\theta^c) < -c_{b,n}\} \\
&\leq \sum_{n=\tau_i^*+1}^{\infty} \mathbb{P}\left\{\{\hat{H}_{b,n} - H_b(\theta^c) < -c_{b,n}\} \cap B_n\right\} + \sum_{n=\tau_i^*+1}^{\infty} \mathbb{P}(B_n^c),
\end{aligned}$$

where the first term is  $\leq \alpha$  since  $B_n \subseteq A_{u^*}$ , and for the second term,

$$\begin{aligned} \sum_{n=\tau_i^*+1}^{\infty} \mathbb{P}(B_n^c) &\leq \sum_{n=\tau_i^*+1}^{\infty} \sum_{\ell=n_\eta+1}^n 2d \exp\left(-\frac{\ell(u^*)^2}{2d\bar{\nu}^2}\right) \\ &\leq 2d \sum_{n=\tau_i^*+1}^{\infty} n \exp\left(-\frac{(n_\eta+1)(u^*)^2}{2d\bar{\nu}^2}\right) \\ &\leq 2d \sum_{n=1}^{\infty} n \exp(-\mathcal{K}n), \end{aligned}$$

where  $\mathcal{K} := \eta(u^*)^2/(2d\bar{\nu}^2)$ . By a direct computation, we have

$$\sum_{n=1}^{\infty} n \exp(-\mathcal{K}n) = \sum_{n=1}^{\infty} \sum_{m=1}^n \exp(-\mathcal{K}n) = \sum_{m=1}^{\infty} \sum_{n=m}^{\infty} \exp(-\mathcal{K}n) = \frac{e^{-\mathcal{K}}}{(1 - e^{-\mathcal{K}})^2}.$$

We therefore conclude that  $\sum_{n=\tau_i^*+1}^{\infty} \mathbb{P}(B_n^c) \leq 2de^{-\mathcal{K}}(1 - e^{-\mathcal{K}})^{-2}$ . Putting all the bounds together yields (4.2.8).  $\square$

#### 4.2.4 The Pairwise SE-IU Algorithm

Despite the elegance of the Sequential Elimination framework, it overlooks two important factors in stochastic simulation: (i) as a variance reduction technique, common random numbers (CRN), i.e., sharing the same  $\{\xi_{ir}\}_r$  across all designs, often sharpens the comparison between designs; (ii) the common input distribution is another form of CRN, except that it is beyond our control. The best way to exploit these factors is to use pairwise comparisons, i.e., comparing each pair of designs, and eliminate a design whenever it is clearly dominated by another one. Pairwise comparison is fairly common in traditional R&S algorithms (e.g., KN), but it has not been explored in the context of Sequential Elimination. We will show that, with a slight modification, SE-IU can be compatible with pairwise comparisons, and it can substantially enhance selection efficiency.

Define  $\hat{\delta}_{ij,n} := \hat{H}_{i,n} - \hat{H}_{j,n}$ . Suppose that for any pair of designs  $(i, j)$ , we can find

confidence bounds  $\{c_{ij,n}\}$  such that

$$\mathbb{P} \left\{ |\hat{\delta}_{ij,n} - \delta_{ij}(\theta^c)| \leq c_{ij,n}, \forall n \right\} \geq 1 - \frac{2\alpha}{K(K-1)}, \quad (4.2.9)$$

where  $\alpha \in (0, 1)$  and  $K \geq 2$ . Then, we can design the following elimination rule: if  $\hat{\delta}_{ij,n} > c_{ij,n}$ , then we eliminate design  $j$ ; otherwise if  $\hat{\delta}_{ij,n} < -c_{ij,n}$ , then we eliminate design  $i$ .

**Proposition 4.2.1.** *Assume that (4.2.9) holds for any pair of designs  $(i, j)$ ,  $c_{ij,n} = c_{ji,n}$  for all  $n$ , and  $c_{ij,n} \rightarrow 0$  as  $n \rightarrow \infty$ . Then, the pairwise elimination rule guarantees that  $PCS \geq 1 - \alpha$ .*

*Proof.* Consider the event

$$E := \bigcap_{i=1}^K \bigcap_{j=i+1}^K \bigcap_{n=1}^{\infty} \left\{ |\hat{\delta}_{ij,n} - \delta_{ij}(\theta^c)| \leq c_{ij,n} \right\}.$$

By (4.2.9) and a union bound, we have  $\mathbb{P}(E) \geq 1 - \alpha$ , so it suffices to show that a correct selection happens almost surely on  $E$ . For any pair of designs  $i$  and  $j$ , assume without loss of generality that  $\delta_{ij}(\theta^c) > 0$ . First, notice that on  $E$ ,

$$\hat{\delta}_{ij,n} > \hat{\delta}_{ij,n} - \delta_{ij}(\theta^c) \geq -c_{ij,n}, \quad \forall n,$$

so design  $i$  will never get eliminated by design  $j$ . Moreover, since  $c_{ij,n} \rightarrow 0$  as  $n \rightarrow \infty$ , there exists a positive constant  $N$  such that  $c_{ij,N} < \delta_{ij}(\theta^c)/2$ . If design  $j$  has not been eliminated in the first  $N - 1$  stages, then at the  $N$ th stage,

$$\hat{\delta}_{ij,N} \geq \delta_{ij}(\theta^c) - c_{ij,N} > \delta_{ij}(\theta^c)/2 > c_{ij,N},$$

which means that design  $j$  will be eliminated. Therefore, all the inferior designs will be eliminated on event  $E$ . □

In light of Proposition 4.2.1, a valid algorithm can be designed by constructing confidence bounds  $\{c_{ij,n}\}$  satisfying (4.2.9). For any pair of designs  $(i, j)$ , let  $\sigma_{ij}^2(\theta) := \text{Var}_{P_\theta}[h_i(\xi) - h_j(\xi)]$ , and assume that there is a function  $L_{ij}(\cdot)$  such that

$$|\delta_{ij}(\theta_1) - \delta_{ij}(\theta_2)| \leq L_{ij}(u) \|\theta_1 - \theta_2\|, \quad \forall \theta_1, \theta_2 \in \{\theta \in \Theta \mid \|\theta - \theta^c\| \leq u\}.$$

We have the following pairwise version of SE-IU.

*Algorithm: Pairwise SE-IU (ideal version)*

- **Input.**  $\alpha \in (0, 1), \eta \in (0, 1), K \geq 2, n_0 \geq 10$ .
- **Step 1.** Solve the following equation in  $u$ , and let  $u^*$  be the solution.

$$\sum_{j=1}^d \frac{\exp\left(-\frac{(n_0+1)u^2}{2d\nu_j^2}\right)}{1 - \exp\left(-\frac{u^2}{2d\nu_j^2}\right)} = \frac{\alpha}{6}.$$

- **Step 2.** For each design, compute

$$\bar{\sigma}_{ij} := \sup_{\substack{\|\theta - \theta^c\| \leq u^* \\ \theta \in \Theta}} \sigma_{ij}(\theta), \quad \bar{L}_{ij} := L_{ij}(u^*),$$

as well as the constants

$$\kappa_{n_0} := \sum_{n=n_0+1}^{\infty} n^{-2}, \quad \beta_{n_0} := \sum_{n=n_0+1}^{\infty} (n - n_\eta)^{-2}.$$

Let  $\bar{\nu} := \max_j \nu_j$ . Run  $n_0$  stages and set  $n \leftarrow n_0 + 1$ . Also let  $\mathcal{S} \leftarrow \{1, 2, \dots, K\}$ .

- **Step 3.** Run an additional stage for all designs  $\{1, 2, \dots, K\}$  using CRN, and compute their estimates  $\hat{H}_{i,n}$  using the moving average estimator in (4.2.1).



- **Step 4.** For any pair of surviving designs  $i$  and  $j$ , compute  $c_{ij,n} = t_{ij,n} + r_{ij,n}$ , where

$$\begin{aligned} t_{ij,n} &:= 2\bar{\sigma}_{ij} \sqrt{\frac{\ln \left( \sqrt{\frac{3K(K-1)\kappa_{n_0}}{\alpha}} n \right)}{n - n_\eta}}, \\ r_{ij,n} &:= \bar{\nu} \bar{L}_{ij} \sqrt{\frac{6d \ln \left( \left( \frac{3dK(K-1)\beta_{n_0}}{\alpha} \right)^{\frac{1}{3}} (n - n_\eta) \right)}{n_\eta + 1}}. \end{aligned} \quad (4.2.10)$$

Set  $\mathcal{S} \leftarrow \mathcal{S} \setminus \{i\}$  (or  $\mathcal{S} \leftarrow \mathcal{S} \setminus \{j\}$ ) if  $\hat{\delta}_{ij,n} > c_{ij,n}$ , (or  $\hat{\delta}_{ij,n} < -c_{ij,n}$ ). Go to Output if  $|\mathcal{S}| = 1$ ; otherwise, set  $n \leftarrow n + 1$  and go to Step 3.

- **Output.** Select the only design in  $\mathcal{S}$  as the best one.

The Pairwise SE-IU algorithm is almost identical to SE-IU, except that the confidence bounds  $\{c_{ij,n}\}$  are computed based on  $\sigma_{ij}$  and  $L_{ij}$ , instead of  $\sigma_i$  and  $L_i$ . We argue that this difference is the key to faster stopping. Indeed, with a slight abuse of notation, SE-IU is equivalent to pairwise comparison with  $c_{ij,n} = c_{i,n} + c_{j,n}$ . However, the confidence bounds in Pairwise SE-IU tend to be much narrower, since (i) we typically have  $\sigma_{ij} < \sigma_i + \sigma_j$  due to CRN; (ii) the common input distribution effect often results in  $L_{ij} < L_i + L_j$ . Similar to SE-IU, we provide the following theoretical guarantee for Pairwise SE-IU.

**Theorem 4.2.3.** *Let Assumption 4.2.2 hold. Then, the Pairwise SE-IU algorithm guarantees to select the best design with probability at least  $1 - \alpha$ . Furthermore,*

$$\mathbb{E}[\tau^*] \leq 2 \sum_{i \neq b} \tau_i^* + 2(K-1)(\alpha + 2de^{-\mathcal{K}}(1 - e^{-\mathcal{K}})^{-2}),$$

where  $\tau_i^* := \inf\{n > n_0 \mid 2c_{bi,n} \leq \delta_{bi}(\theta^e)\}$  and  $\mathcal{K} := \eta(u^*)^2/(2d\bar{\nu}^2)$ .

*Proof.* Notice that under Assumption 4.2.2,  $h_i(\xi) - h_j(\xi)$  is again sub-Gaussian, and  $L_{ij}$  is guaranteed to exist ( $L_{ij}(u) \leq L_i(u) + L_j(u)$ ). The rest of the proof is almost identical to that of Theorem 4.2.2 and is therefore omitted.  $\square$

If CRN and the common input distribution effect achieve variance reduction (which is often the case in practice), then the  $\tilde{\tau}_i$  in Theorem 4.2.3 is much smaller than the  $\tau_i^*$  in Theorem 4.2.2. Thus, the advantage of Pairwise SE-IU is also reflected in the upper bound on  $\mathbb{E}[\tilde{\tau}]$ .

#### 4.2.5 A Heuristic Algorithm

The SE-IU and Pairwise SE-IU algorithms are usually conservative, so we further propose a heuristic algorithm that works well in practice. The idea is to construct pairwise confidence bounds  $\tilde{c}_{ij,n}$  approximately using our asymptotic normality result for the moving average estimator. By a straightforward extension of Theorem 4.2.1, we have that

$$\sqrt{n}[\hat{\delta}_{ij,n} - \delta_{ij}(\theta^c)] \Rightarrow \mathcal{N}(0, \tilde{\sigma}_{ij,\infty}^2), \quad \text{as } n \rightarrow \infty,$$

where

$$\tilde{\sigma}_{ij,\infty}^2 := w_\eta \nabla \delta_{ij}(\theta^c)^\top \Sigma_G \nabla \delta_{ij}(\theta^c) + \frac{1}{1-\eta} \sigma_{ij}^2(\theta^c),$$

and

$$w_\eta := \frac{2}{1-\eta} + \frac{2\eta \log \eta}{(1-\eta)^2}.$$

Therefore, we may view  $\hat{\delta}_{ij,n} - \delta_{ij}(\theta^c)$  as approximately distributed as  $\mathcal{N}(0, \tilde{\sigma}_{ij,\infty}/\sqrt{n})$ . If this were accurate, then using the following confidence bounds,

$$\tilde{c}_{ij,n} = 2\tilde{\sigma}_{ij,\infty} \sqrt{\frac{\ln \left( \sqrt{\frac{K(K-1)\pi^2}{6\alpha}} \right) n}{n}},$$

we would have

$$\begin{aligned} \text{PFS} &\leq \sum_{i=1}^K \sum_{j=i+1}^K \sum_{n=1}^{\infty} \mathbb{P} \left\{ |\hat{\delta}_{ij,n} - \delta_{ij}(\theta^c)| > \tilde{c}_{ij,n} \right\} \\ &\leq \sum_{i=1}^K \sum_{j=i+1}^K \sum_{n=1}^{\infty} 2 \exp \left( -\frac{n\tilde{c}_{ij,n}^2}{2\tilde{\sigma}_{ij,\infty}^2} \right) < \alpha, \end{aligned}$$

by a Gaussian tail bound. Of course, the approximation is not accurate for  $n$  being small, and no theoretical guarantee can be provided on its performance. Nonetheless, its practical advantage will be demonstrated numerically in Section 4.4.

#### 4.2.6 Implementation Guidance

We briefly discuss how to estimate the unknown quantities in all three fixed confidence algorithms we proposed. One may start off by collecting a small size of input data for initial estimation. If IU or SU is high (relative to the estimates of  $\delta_{ij}(\theta^c)$ ), then consider using a larger  $n_0$  for SE-IU and Pairwise SE-IU. The case for the heuristic algorithm is straightforward. In SE-IU, the difficult parameters are  $\bar{\sigma}_i$  and  $\bar{L}_i$ , which are the suprema of  $\sigma_i(\cdot)$  and  $\|\nabla H_i(\cdot)\|$  over a small neighborhood of  $\theta^c$ . While one can attempt to maximize the corresponding likelihood ratio estimators, we suggest simply replacing them with estimates of  $\sigma_i(\theta^c)$  and  $\|\nabla H_i(\theta^c)\|$  for the following reasons: (i) estimates based on such maximization often suffer from high variance and severe overestimation; (ii) the Sequential Elimination framework is already conservative since it resorts to loose union bounds, so highly accurate estimates are most likely unnecessary. The same is also recommended for Pairwise SE-IU.

### 4.3 Fixed Budget Formulation

#### 4.3.1 Problem Setup

In this section, we consider a fixed budget setting where acquiring additional data is possible, albeit at some cost (see Section 1.1.1 for examples). Suppose that there is a total

budget  $T$ , which can be used to collect input data as well as run simulation experiments. For simplicity, assume that the cost per data sample for the  $q$ th input distribution is  $c_{D,q}$ , and the cost per simulation run is  $c_S$  (“ $D$ ” for “Data”, and “ $S$ ” for “Simulation”). As is mentioned in Section 1.2.3, the budget could be time or money, as long as  $c_D$  and  $c_S$  are measured in the same unit and are on comparable scales. The goal is to maximize the PCS by wisely allocating the budget between data collection and simulation experimentation.

The problem we described is a two-stage decision-making problem. In the first stage, we decide how much data to collect, and estimate the input distributions. In the second stage, simulations are used to select the best design under the estimated input distributions. There is a clear tradeoff between IU and SU: while collecting excessive data leaves little budget for running simulations, insufficient input data leads to high IU that cannot be reduced by simulation effort. Due to the extra layer of uncertainty, this problem is at least as difficult as traditional fixed budget R&S, and one can only hope to solve it approximately. In the upcoming section, we develop an approximate solution that allows a closed form of the quantity of input data to collect (for each individual input distribution).

#### 4.3.2 An Approximate Solution

Using the OCBA framework, we derive an approximate solution to our fixed budget R&S problem. Let  $N_q$  be the number of input data samples we collect for the  $q$ th distribution, and let  $M_i$  be the number of simulation runs allocated to design  $i$ . For convenience, let  $\mathbf{N} := [N_1, N_2, \dots, N_Q]^\top$  and  $\mathbf{M} := [M_1, M_2, \dots, M_K]^\top$ . Also let  $\hat{\theta}_{\mathbf{N}} := [\hat{\theta}_{N_1}(1)^\top, \dots, \hat{\theta}_{N_Q}(Q)^\top]^\top$  be the estimates of  $\theta^c$ . Different from Assumption 4.2.1, here we do not assume specific structure on  $\hat{\theta}_{\mathbf{N}}$ . The problem described in Section 4.3.1 is an intractable stochastic dynamic program (see [49] for insights from this perspective), and thus is simplified as the

following static optimization problem,

$$\begin{aligned}
\max_{\mathbf{N}, \mathbf{M}} \text{PCS} &:= \mathbb{P} \left\{ \bigcap_{i \neq b} \left\{ \hat{\delta}_{bi}(\hat{\theta}_{\mathbf{N}}) > 0 \right\} \right\} \\
\text{s.t. } &\sum_{q=1}^Q c_{D,q} N_q + c_S \sum_{i=1}^K M_i = T, \\
&N_q \in \mathbb{Z}^+, M_i \in \mathbb{Z}^+, \quad \forall q, i,
\end{aligned} \tag{P1}$$

where  $\mathbb{Z}^+$  denotes the set of all positive integers. Since the PCS does not have a closed form, it is usually approximated by the Bonferroni inequality,

$$\text{PCS} \geq 1 - \sum_{i \neq b} \mathbb{P} \left\{ \hat{\delta}_{bi}(\hat{\theta}_{\mathbf{N}}) \leq 0 \right\}, \tag{4.3.1}$$

where the right-hand side (RHS) of (4.3.1) is referred to as the approximate PCS (APCS). In OCBA's framework,  $\hat{\delta}_{bi}(\theta^c)$  can be roughly viewed as normally distributed due to CLT. When there is IU, CLT is not applicable and a new asymptotic result is in need. The following assumption is made for this purpose, where “ $\Rightarrow$ ” denotes convergence in distribution,  $\|\cdot\|$  is the Euclidean norm, and  $\mathcal{N}$  denotes a normal distribution.

**Assumption 4.3.1.**

- (1) For any  $1 \leq q \leq Q$ ,  $\sqrt{n}(\hat{\theta}_n(q) - \theta^c(q)) \Rightarrow \mathcal{N}(0, \Sigma_{\theta^c(q)})$  as  $n \rightarrow \infty$  for some positive definite covariance matrix  $\Sigma_{\theta^c(q)}$ .
- (2)  $P_\theta$  has a density  $f_\theta(\xi)$  that is differentiable w.r.t.  $\theta$  for all  $\xi \in \mathbb{R}^{m_q}$ .
- (3)  $\int [h_i(\xi)]^2 f_\theta(\xi) d\xi < \infty, \forall \theta \in \Theta, i \in \mathcal{I}$ .
- (4) For almost all  $\xi$  (up to a set of Lebesgue measure 0),

$$|f(\xi; \theta_1) - f(\xi; \theta_2)| \leq L(\xi) \|\theta_1 - \theta_2\|, \quad \forall \theta_1, \theta_2 \in \Theta,$$

where  $\int |h_i(\xi)| L(\xi) < \infty, \int [h_i(\xi)]^2 L(\xi) < \infty, \forall i \in \mathcal{I}$ .

In Assumption 4.3.1, (1) holds for many estimators. For example, the maximum likelihood estimator satisfies (1) with  $\Sigma_{\theta^c(q)}$  being the inverse of Fisher information; (2) also holds for many parametric families. If instead  $P_\theta$  is a discrete distribution, then all integrals can easily be replaced by summations; (3) ensures that the first two moments of  $h_i(\xi)$  are well-defined; (4) is a commonly imposed Lipschitz-type condition, which together with the Dominated Convergence Theorem implies that

$$\begin{aligned}\partial_\theta \int h_i(\xi) f(\xi; \theta) d\xi &= \int h_i(\xi) \partial_\theta f(\xi; \theta) d\xi, \\ \partial_\theta \int [h_i(\xi)]^2 f(\xi; \theta) d\xi &= \int [h_i(\xi)]^2 \partial_\theta f(\xi; \theta) d\xi.\end{aligned}$$

In the following theorem,  $\mathbf{N}$  and  $\mathbf{M}$  are viewed as deterministic functions of  $T$ .

**Theorem 4.3.1.** *Let Assumption 4.3.1 hold. If there exists positive constants  $\rho_1, \rho_2, \dots, \rho_Q$  and  $\pi_1, \pi_2, \dots, \pi_K$  such that  $N_q/T \rightarrow \rho_q$  and  $M_i/T \rightarrow \pi_i$  as  $T \rightarrow \infty$ , then for any two designs  $i$  and  $j$ ,*

$$\sqrt{T} \left[ \hat{\delta}_{ij}(\hat{\theta}_{\mathbf{N}}) - \delta_{ij}(\theta^c) \right] \Rightarrow \mathcal{N}(0, \sigma_{ij,\infty}^2) \quad \text{as } T \rightarrow \infty,$$

where

$$\sigma_{ij,\infty}^2 := \sum_{q=1}^Q \frac{\psi_{ij}^2(q)}{\rho_q} + \frac{\sigma_i^2(\theta^c)}{\pi_i} + \frac{\sigma_j^2(\theta^c)}{\pi_j},$$

and

$$\psi_{ij}^2(q) := V_{ij}^{(q)}(\theta^c)^\top \Sigma_{\theta^c(q)} V_{ij}^{(q)}(\theta^c), \quad V_{ij}^{(q)}(\theta) := \frac{\partial \delta_{ij}(\theta)}{\partial \theta(q)}.$$

*Proof of Theorem 4.3.1.* We work with the following decomposition.

$$\sqrt{T} \left[ \hat{\delta}_{ij}(\hat{\theta}_{\mathbf{N}}) - \delta_{ij}(\theta^c) \right] = \underbrace{\sqrt{T} \left[ \hat{\delta}_{ij}(\hat{\theta}_{\mathbf{N}}) - \delta_{ij}(\hat{\theta}_{\mathbf{N}}) \right]}_{X_T} + \underbrace{\sqrt{T} \left[ \delta_{ij}(\hat{\theta}_{\mathbf{N}}) - \delta_{ij}(\theta^c) \right]}_{Y_T}$$

Let  $\mathbf{i}$  denote the imaginary number  $\sqrt{-1}$ . For any  $t \in \mathbb{R}$ , we have

$$\mathbb{E}[e^{\mathbf{i}t(X_T+Y_T)}] = \mathbb{E}\left\{\mathbb{E}[e^{\mathbf{i}t(X_T+Y_T)} \mid \hat{\theta}_{\mathbf{N}}]\right\} = \mathbb{E}\left\{e^{\mathbf{i}tY_T}\mathbb{E}[e^{\mathbf{i}tX_T} \mid \hat{\theta}_{\mathbf{N}}]\right\}$$

The rest of the proof is carried out in the following steps.

(i)  $Y_T \Rightarrow \mathcal{N}\left(0, \sum_{q=1}^Q \frac{\psi_{ij}^2(q)}{\rho_q}\right)$  as  $T \rightarrow \infty$ .

Due to Assumption 4.3.1 (i), we have  $\sqrt{T}(\hat{\theta}_{\mathbf{N}} - \theta^c) \Rightarrow \mathcal{N}(0, \tilde{\Sigma})$  as  $T \rightarrow \infty$ , where  $\tilde{\Sigma} := \text{blkdiag}\left(\Sigma_{\theta^c(1)}/\rho_1, \dots, \Sigma_{\theta^c(Q)}/\rho_Q\right)$  and “blkdiag” denotes a block diagonal matrix. Then, the convergence follows from the Delta Theorem (see, e.g., [90]).

(ii)  $\mathbb{E}[e^{\mathbf{i}tX_T} \mid \hat{\theta}_{\mathbf{N}}] \Rightarrow \exp(-\sigma_i^2(\theta^c)t^2/2\pi_i)$  as  $T \rightarrow \infty$ .

Note that conditioned on  $\hat{\theta}_{\mathbf{N}}$ ,  $Z_{ir}(\hat{\theta}_{\mathbf{N}}) := h_i(\xi_{ir}) - H_i(\hat{\theta}_{\mathbf{N}})$ ,  $r = 1, 2, \dots, M_i$  are i.i.d. random variables with mean 0 and variance  $\sigma_i^2(\hat{\theta}_{\mathbf{N}})$ . Thus, it can be checked that

$$\mathbb{E}[e^{\mathbf{i}tX_T} \mid \hat{\theta}_{\mathbf{N}}] = \left[\phi_{Z_{i1}(\hat{\theta}_{\mathbf{N}})}\left(\frac{t\sqrt{T}}{M_i}\right)\right]^{M_i} \cdot \left[\phi_{Z_{j1}(\hat{\theta}_{\mathbf{N}})}\left(-\frac{t\sqrt{T}}{M_j}\right)\right]^{M_j},$$

where  $\phi_X(\cdot)$  denotes the characteristic function of  $X$ . Furthermore, by Theorem 3.3.8 from [63],

$$\phi_{Z_{i1}(\hat{\theta}_{\mathbf{N}})}\left(\frac{t\sqrt{T}}{M_i}\right) = 1 - \sigma_i^2(\hat{\theta}_{\mathbf{N}})\frac{t^2}{2M_i}\frac{T}{M_i} + o\left(\frac{1}{M_i}\right).$$

Since  $\hat{\theta}_{\mathbf{N}} \Rightarrow \theta^c$ ,  $\sigma_i^2(\hat{\theta}_{\mathbf{N}}) \Rightarrow \sigma_i^2(\theta^c)$  by the continuity of  $\sigma_i^2(\cdot)$ , and

$$\sigma_i^2(\hat{\theta}_{\mathbf{N}})\frac{t^2}{2}\frac{T}{M_i} \Rightarrow \frac{\sigma_i^2(\theta^c)t^2}{2\pi_i} \quad \text{as } T \rightarrow \infty.$$

Let  $\mathbb{C}$  denote the set of all complex numbers. Using the fact that if  $c_n \rightarrow c \in \mathbb{C}$ , then

$(1 + c_n/n)^n \rightarrow e^c$  as  $n \rightarrow \infty$ , we further have

$$\left[ \phi_{Z_{i1}(\hat{\theta}_{\mathbf{N}})} \left( \frac{t\sqrt{T}}{M_i} \right) \right]^{M_i} \Rightarrow \exp \left( -\frac{\sigma_i^2(\theta^c)t^2}{2\pi_i} \right) \quad \text{as } T \rightarrow \infty.$$

(iii) Combining observations (i) and (ii) together with the Dominated Convergence Theorem (since the integrand is dominated by 1), we have

$$\mathbb{E}[e^{it(X_T+Y_T)}] \rightarrow \exp \left( -\sum_{q=1}^Q \frac{\psi_{ij}^2(q)t^2}{2\rho_q} \right) \exp \left( -\frac{\sigma_i^2(\theta^c)t^2}{2\pi_i} \right) \exp \left( -\frac{\sigma_j^2(\theta^c)t^2}{2\pi_j} \right),$$

which implies the desired result. □

Theorem 4.3.1 echoes a classical result in [3] for a single design with a single input distribution (i.e.,  $Q = 1, \mathbf{N} = N_1$ ), which states that

$$\text{Var}[\hat{H}_i(\hat{\theta}_{N_1})] = \frac{\nabla H_i(\theta^c)^\top \Sigma_{\theta^c(1)} \nabla H_i(\theta^c)}{N_1} + \frac{\sigma_i^2(\theta^c)}{M_i} + \mathcal{R},$$

where  $\mathcal{R} \rightarrow 0$  as  $N_1$  and  $M_i$  tend to infinity. In other words, the variance of  $\hat{H}_i(\hat{\theta}_{N_1})$  can be decomposed into two parts corresponding to IU and SU, respectively. Our result not only extends it to multiple independent input distributions, but also characterizes the asymptotic distribution of  $\hat{\delta}_{ij}(\hat{\theta}_{N_1})$ , which will be useful for approximating the APCS.

Some insights can be developed on why the linear asymptotic regime (i.e.,  $N_q/T \rightarrow \rho_q, M_i/T \rightarrow \pi_i$ ) is crucial. For simplicity, consider the case of  $Q = 1$ . Notice that for a design  $i$ , we have the following decomposition.

$$\sqrt{N_1}[\hat{H}_i(\hat{\theta}_{N_1}) - H_i(\theta^c)] = \underbrace{\sqrt{N_1}[\hat{H}_i(\hat{\theta}_{N_1}) - H_i(\hat{\theta}_{N_1})]}_{(*)} + \underbrace{\sqrt{N_1}[H_i(\hat{\theta}_{N_1}) - H_i(\theta^c)]}_{(**)}, \quad (4.3.2)$$

where  $(*)$  captures SU and  $(**)$  captures IU. For  $(**)$ , the Delta Theorem (see, e.g., [90])



can be applied to get

$$\sqrt{N_1}[H_i(\hat{\theta}_{N_1}) - H_i(\theta^c)] \Rightarrow \nabla H_i(\theta^c)^\top \mathcal{N}(0, \Sigma_{\theta^c(1)}) \quad \text{as } N_1 \rightarrow \infty.$$

For (\*), it is possible to use the characteristic function to show that

$$\sqrt{M_i}[\hat{H}_i(\hat{\theta}_{N_1}) - H_i(\hat{\theta}_{N_1})] \Rightarrow \mathcal{N}(0, \sigma_i^2(\theta^c)) \quad \text{as } M_i \rightarrow \infty,$$

provided that  $N_1, M_i \rightarrow \infty$  simultaneously. If  $N_1/M_i \rightarrow 0$  as  $N_1 \rightarrow \infty$ , the RHS of (4.3.2) can be rewritten as

$$\sqrt{\frac{N_1}{M_i}} \sqrt{M_i}[\hat{H}_i(\hat{\theta}_{N_1}) - H_i(\hat{\theta}_{N_1})] + \sqrt{N_1}[H_i(\hat{\theta}_{N_1}) - H_i(\theta^c)],$$

where the first term converges to 0 in probability, and the sum converges in distribution to  $\nabla H_i(\theta^c)^\top \mathcal{N}(0, \Sigma_{\theta^c(1)})$  as  $N_1 \rightarrow \infty$ , meaning that IU dominates SU. A symmetric conclusion can also be drawn for the case of  $M_i/N_1 \rightarrow 0$ .

We now use Theorem 4.3.1 to derive an approximate solution to (P1). By Theorem 4.3.1, we have  $\hat{\delta}_{ij}(\hat{\theta}_N) \stackrel{\mathcal{D}}{\approx} \mathcal{N}(\delta_{ij}(\theta^c), \Psi_{ij}^2)$ , where  $\stackrel{\mathcal{D}}{\approx}$  stands for “approximately distributed as”, and

$$\Psi_{ij}^2 := \frac{\sigma_{ij,\infty}^2}{T} \approx \sum_{q=1}^Q \frac{\psi_{ij}^2(q)}{N_q} + \frac{\sigma_i^2(\theta^c)}{M_i} + \frac{\sigma_j^2(\theta^c)}{M_j}.$$

For simplicity, we will drop  $\theta^c$  when there is no ambiguity. Since  $\text{PCS} \geq 1 - \sum_{i \neq b} \mathbb{P}\left\{\hat{\delta}_{bi}(\hat{\theta}_N) \leq 0\right\}$ , we can approximate the APCS as

$$\widehat{\text{APCS}} = 1 - \sum_{i \neq b} \int_{-\infty}^{-\frac{\delta_{bi}}{\Psi_{bi}}} \frac{1}{\sqrt{2\pi}} e^{-\frac{t^2}{2}} dt.$$

Following the OCBA framework, we further drop the integrality and nonnegativity con-

straints on  $N_q$  and  $M_i$ . Using the Lagrangian function

$$\mathcal{L} := \widehat{\text{APCS}} + \lambda \left( \sum_{q=1}^Q c_{D,q} N_q + c_S \sum_{i=1}^K M_i - T \right),$$

we have the following KKT conditions.

$$\frac{\partial \mathcal{L}}{\partial N_q} = c_{D,q} \lambda - \sum_{i \neq b} \frac{1}{2\sqrt{2\pi}} \exp \left( -\frac{\delta_{bi}^2}{2\Psi_{bi}^2} \right) \frac{\delta_{bi} \psi_{bi}^2(q)}{\Psi_{bi}^3 N_q^2} = 0, \quad (4.3.3)$$

$$\frac{\partial \mathcal{L}}{\partial M_i} = c_S \lambda - \frac{1}{2\sqrt{2\pi}} \exp \left( -\frac{\delta_{bi}^2}{2\Psi_{bi}^2} \right) \frac{\delta_{bi} \sigma_i^2}{\Psi_{bi}^3 M_i^2} = 0 \quad \forall i \neq b, \quad (4.3.4)$$

$$\frac{\partial \mathcal{L}}{\partial M_b} = c_S \lambda - \sum_{i \neq b} \frac{1}{2\sqrt{2\pi}} \exp \left( -\frac{\delta_{bi}^2}{2\Psi_{bi}^2} \right) \frac{\delta_{bi} \sigma_b^2}{\Psi_{bi}^3 M_b^2} = 0, \quad (4.3.5)$$

$$\sum_{q=1}^Q c_{D,q} N_q + c_S \sum_{i=1}^K M_i = T. \quad (4.3.6)$$

From (4.3.4) we have

$$\frac{1}{2\sqrt{2\pi}} \exp \left( -\frac{\delta_{bi}^2}{2\Psi_{bi}^2} \right) \frac{\delta_{bi}}{\Psi_{bi}^3} = c_S \lambda \frac{M_i^2}{\sigma_i^2},$$

and plugging it into (4.3.3) yields

$$N_q = \sqrt{\frac{c_S}{c_{D,q}} \sum_{i \neq b} \frac{M_i^2 \psi_{bi}^2(q)}{\sigma_i^2}}, \quad \forall 1 \leq q \leq Q, \quad (4.3.7)$$

which provides a closed-form solution of  $N_q$ .

A few remarks on (4.3.7) are made as follows. First, the optimal  $N_q$  depends on the cost ratio  $c_S/c_D$ : the cheaper data is relative to simulation, the more data we should collect. Second,  $N_q$  is related to the squared sum of  $\{M_i\}$  weighted by  $\psi_{bi}^2(q)/\sigma_i^2$ . Note that  $\psi_{bi}^2(q)$  depends on  $\partial \delta_{ij}(\theta)/\partial \theta(q)$ , which captures the relative sensitivity of designs  $b$  and  $i$ 's difference in expected performance with respect to the estimation error in  $\hat{\theta}_{\mathbf{N}}$ .

The relative sensitivity information also appeared in [56] as a way to exploit the com-

mon input distribution effect. For a quick intuition, consider a special case where there exist constants  $C_i$  such that  $H_i(\theta) = C_i + \theta$ . As  $\theta$  varies, every design's expected performance shifts by the same amount, and their relative order will never be perturbed. Data collection is unnecessary in this case since plugging in any  $\theta \in \Theta$  would suffice. This coincides with the result yielded by (4.3.7), since  $\partial\delta_{ij}(\theta)/\partial\theta(q) = 0$  for any pair of designs  $i$  and  $j$ . Similarly, a large  $\psi_{bi}^2(q)$  relative to  $\sigma_i^2$  suggests that  $\delta_{ij}(\cdot)$  is very sensitive to the estimation error of  $\hat{\theta}_N$ , and a larger  $N_q$  should be anticipated.

While the solution for  $\{M_i\}$  does not seem to admit a closed form, in principle the KKT conditions (4.3.3) - (4.3.6) can be solved using any off-the-shelf commercial solver. For a fast heuristic solution, one may turn to the well-known OCBA allocation rule (see (4.3.8) in Section 4.3.3).

#### 4.3.3 The OCBAIU Algorithm

With the closed form solution of  $N_q$  in (4.3.7), we can compute  $\mathbf{N}$  and  $\mathbf{M}$  by plugging in estimates of  $H_i(\theta^c)$ ,  $\sigma_i^2(\theta^c)$  and  $\psi_{ij}^2$ . However, directly implementing the resulting  $\mathbf{N}$  and  $\mathbf{M}$  is not necessarily the best practice. Observe that the PCS can be decomposed as

$$\text{PCS} = \mathbb{P}\{\hat{b} = b \mid \hat{\theta}_N \in \mathcal{P}\} \cdot \mathbb{P}\{\hat{\theta}_N \in \mathcal{P}\} + \mathbb{P}\{\hat{b} = b \mid \hat{\theta}_N \notin \mathcal{P}\} \cdot \mathbb{P}\{\hat{\theta}_N \notin \mathcal{P}\},$$

where  $\hat{b}$  is the estimated best design and  $\mathcal{P}$  is the perturbation region defined in (4.1.2). If  $\hat{\theta}_N$  falls in  $\mathcal{P}$ , then no reasonable algorithm is expected to deliver a good  $\mathbb{P}\{\hat{b} = b \mid \hat{\theta}_N \in \mathcal{P}\}$ . Thus, the only hope is to maximize  $\mathbb{P}\{\hat{b} = b \mid \hat{\theta}_N \notin \mathcal{P}\}$ . But if  $\hat{\theta}_N \notin \mathcal{P}$ , then the second-stage problem reduces to the traditional R&S without IU, where existing algorithms apply readily. In this chapter, we build on the OCBA algorithm, which asymptotically implements the following allocation rule

$$M_b = \sigma_b \sqrt{\sum_{i \neq b} \frac{M_i^2}{\sigma_i^2}}, \quad \frac{M_i}{M_j} = \frac{\sigma_i^2 / \delta_{bi}^2}{\sigma_j^2 / \delta_{bj}^2}, \quad i \neq j \neq b, \quad (4.3.8)$$

through dynamic sequential allocation. For more implementation details, we refer the reader to [39, 78] for a full description of the algorithm.

A number of issues need to be addressed when it comes to implementation. First, to obtain initial estimates of  $H_i(\theta^c)$ ,  $\sigma_i^2(\theta^c)$  and  $\psi_{ij}^2$ , we begin by collecting  $N_0$  data samples for each input distribution. The input data can be used to estimate  $\hat{\theta}_{\mathbf{N}}$ , which are also shared across different designs to run simulations for estimating  $H_i(\theta^c)$  and  $\sigma_i^2(\theta^c)$ . In particular, the partial derivatives  $\partial H_i(\theta)/\partial \theta(q)$  can be estimated in many ways. For instance, [56] estimates it by fitting a linear regression model. In this chapter, we use a likelihood ratio estimator

$$\frac{\partial H_i(\theta)}{\partial \theta(q)} \approx \frac{1}{N_0} \sum_{r=1}^{N_0} h_i(\zeta_r) \frac{\partial f_{\theta}(\zeta_r)/\partial \theta(q)}{f_{\theta}(\zeta_r)},$$

where  $\{\zeta_r\}_{r=1}^{N_0}$  are the input data. In addition, we need to decide  $N_0$  and  $M_0$ , where the latter is the size of OCBA's initial simulation runs for each design. As is revealed in Chapter 3 and [91], a budget-independent  $M_0$  can result in a polynomial convergence rate of the probability of false selection (PFS, i.e.,  $1 - \text{PCS}$ ). Therefore, we choose positive constants  $\rho_0$  and  $\pi_0$  and set  $N_0 = \lfloor \rho_0 T \rfloor$  and  $M_0 = \lfloor \pi_0 T \rfloor$ . Our OCBAIU algorithm is presented as follows.

*Algorithm: OCBAIU*

- **Input:**  $\rho_0, \pi_0, T$  and other parameters for OCBA.
- **Initialization:** Collect  $N_0 = \lfloor \rho_0 T \rfloor$  input data samples, compute  $\hat{\theta}_{\mathbf{N}}$  and estimate  $H_i(\theta^c), \sigma_i^2(\theta^c), \partial H_i(\theta)/\partial \theta(q)$  for all designs and all input distributions.
- **Step 1:** Compute  $\mathbf{N}$  using (4.3.7) and (4.3.8). For each input distribution, if  $N_q > N_0$ , then collect additional  $N_q - N_0$  input data and update the estimate of  $\theta^c(q)$ .
- **Step 2:** Run the OCBA algorithm using the remaining budget, where  $M_0 = \lfloor \pi_0 T \rfloor$  and the random samples  $\{\xi_{ir}\}$  are drawn independently from  $P_{\hat{\theta}_{\mathbf{N}}}$ .
- **Output:**  $\hat{b} := \arg \max_{i \in \mathcal{I}} \hat{H}_i(\hat{\theta}_{\mathbf{N}})$ .

Under appropriate regularity conditions, a statistical guarantee can be provided on OCBAIU's finite-sample performance. For each design  $i \neq b$ , let  $z_i > 0$  be a number such that

$$\inf_{\theta \in \Theta, \|\theta - \theta^c\| \leq z_i} \delta_{bi}(\theta) \geq \delta_{bi}(\theta^c)/2, \quad (4.3.9)$$

and let  $z^* := \min_{i \neq b} z_i$ . Since we assume that  $\delta_{bi}(\theta^c) > 0$ , such an  $z_i$  exists by the continuity of  $H_i(\cdot)$  and the closedness of  $\Theta$ . With the following additional assumption, we provide a finite-sample bound on the PFS.

**Assumption 4.3.2.**

- (i) For each  $\hat{\theta}_n(q)$ , there exists functions  $B_q(\cdot) > 0$  and  $C_q(\cdot) > 0$  such that for any  $t > 0$ ,

$$\mathbb{P} \left\{ \|\hat{\theta}_n(q) - \theta^c(q)\| > t \right\} \leq B_q(t) e^{-C_q(t)n}, \quad \forall n \geq 1.$$

- (ii) For any  $\theta \in \Theta$ , if  $\xi \sim P_\theta$ , then for every design  $i$ ,  $h_i(\xi)$  is a sub-Gaussian r.v.

**Theorem 4.3.2.** Let Assumptions 4.3.1 and 4.3.2 hold. Also let  $\bar{\sigma}_i := \sup_{\|\theta - \theta^c\| \leq z^*, \theta \in \Theta} \sigma_i(\theta)$  and  $\bar{C}_q := C_q(z^*/\sqrt{Q})$ . Then, for the OCBA-IU algorithm, there exist positive constants  $\Gamma_1$  and  $\Gamma_2$  (both independent of  $T$ ) such that

$$PFS(T) \leq \Gamma_1 \sum_{q=1}^Q \exp(-\bar{C}_q \lfloor \rho_0 T \rfloor) + \Gamma_2 \sum_{i=1}^K \exp\left(-\frac{\Delta_i^2 \lfloor \pi_0 T \rfloor}{32\bar{\sigma}_i^2}\right), \quad \forall T \geq 0,$$

where  $\Delta_i := \delta_{bi}(\theta^c)$  if  $i \neq b$  and  $\Delta_b := \min_{i \neq b} \Delta_i$ .

Theorem 4.3.2 guarantees an exponential convergence rate of PFS for OCBAIU, which is not surprising since (i)  $\hat{\theta}_n(q)$  and  $h_i(\xi)$  are assumed to be light-tailed; (ii)  $N_0$  and  $M_0$  are required to increase linearly in  $T$ .

*Proof of Theorem 4.3.2.* Let  $E := \bigcap_{q=1}^Q \bigcap_{n=N_0}^\infty \left\{ \|\hat{\theta}_n(q) - \theta^c(q)\| \leq z^*/\sqrt{Q} \right\}$ . Then, we have

$$PFS \leq \mathbb{P}(\text{FS} \cap E) + \mathbb{P}(E^c) \leq \mathbb{P}(\text{FS} \mid E) + \mathbb{P}(E^c),$$

where “FS” denotes the false selection event.

(i) Bounding  $\mathbb{P}(E^c)$ .

$$\begin{aligned}
\mathbb{P}(E^c) &\leq \sum_{q=1}^Q \sum_{n=N_0}^{\infty} \mathbb{P} \left\{ \|\hat{\theta}_n(q) - \theta^c(q)\| > z^*/\sqrt{Q} \right\} \\
&\leq \sum_{q=1}^Q \sum_{n=N_0}^{\infty} B_q(z^*/\sqrt{Q}) e^{-\bar{C}_q n} \\
&\leq \max_q \left\{ \frac{B_q(z^*/\sqrt{Q})}{1 - e^{-\bar{C}_q}} \right\} \sum_{q=1}^Q e^{-\bar{C}_q \lfloor \rho_0 T \rfloor}
\end{aligned}$$

(ii) Bounding  $\mathbb{P}(\text{FS} \mid E)$ .

Note that on event  $E$ , we have  $\|\hat{\theta}_{\mathbf{N}} - \theta^c\| \leq z^*$  almost surely. Moreover, it follows from the definition of  $z^*$  that conditioned on  $E$ ,

$$\bigcap_{i=1}^K \bigcap_{n=M_0}^{\infty} \left\{ |\hat{H}_i(\hat{\theta}_{\mathbf{N}}) - H_i(\hat{\theta}_{\mathbf{N}})| \leq \frac{\Delta_i}{4} \right\} \subseteq \text{CS},$$

where “CS” denotes the correct selection event. Applying a sub-Gaussian bound,

$$\begin{aligned}
\mathbb{P}(\text{FS} \mid E) &\leq \sum_{i=1}^K \sum_{n=M_0}^{\infty} \mathbb{P} \left\{ |\hat{H}_i(\hat{\theta}_{\mathbf{N}}) - H_i(\hat{\theta}_{\mathbf{N}})| > \frac{\Delta_i}{4} \right\} \\
&\leq \max_i \left\{ \frac{2}{1 - \exp\left(-\frac{\Delta_i^2}{32\bar{\sigma}_i^2}\right)} \right\} \sum_{i=1}^K \exp\left(-\frac{\Delta_i^2 \lfloor \pi_0 T \rfloor}{32\bar{\sigma}_i^2}\right),
\end{aligned}$$

where  $\bar{\sigma}_i < \infty$  since  $\sigma_i(\cdot)$  is continuous and  $\{\theta \in \Theta \mid \|\theta - \theta^c\| \leq z^*\}$  is compact.

Defining the constants  $\Gamma_1$  and  $\Gamma_2$  accordingly gives the desired bound.  $\square$

## 4.4 Numerical Results

### 4.4.1 Production-inventory Example

We test our algorithms on a production-inventory problem borrowed from [92]. In this problem, the objective function does not have a closed form and simulation is required for evaluating a design's performance. Suppose that we are running a capacitated production system and we want to minimize the expected total cost over a finite number of periods. The decision variable is the order-up-to level, i.e., the quantity we should fill up to once the inventory falls below that level. Meanwhile, there is an upper bound on the production amount in each period. Within every period, production from the last period arrives first. Then, we observe the demand and fill or backlog them based on the on-hand inventory. Decision of the production amount is carried out at the end of the period. The variables are listed as follows.

1. The order-up-to level:  $s$ .
2. Inventory level at the  $t$ th period:  $I_t$ .
3. Demand at the  $t$ th period:  $\mathcal{D}_t$ .
4. Production amount at the  $t$ th period:  $R_t$ .

Let  $I_0 = s$  and  $R_0 = 0$ . The system dynamics evolve according to the following equations,

$$\begin{aligned} I_{t+1} &= I_t - \mathcal{D}_t + R_{t-1}, \\ R_t &= \min\{R^*, (s - I_{t+1})^+\}, \end{aligned}$$

where  $a^+ := \max\{0, a\}$  and  $R^*$  is the maximum production amount. Assume that the demands are independent random variables, and each  $\mathcal{D}_t$  follows an exponential distribution

with mean  $\theta_t^c$ . Let  $c_H$  be the holding cost per unit and  $c_B$  be the backlog cost per unit. Then, we have the cost at the  $t$ th period as

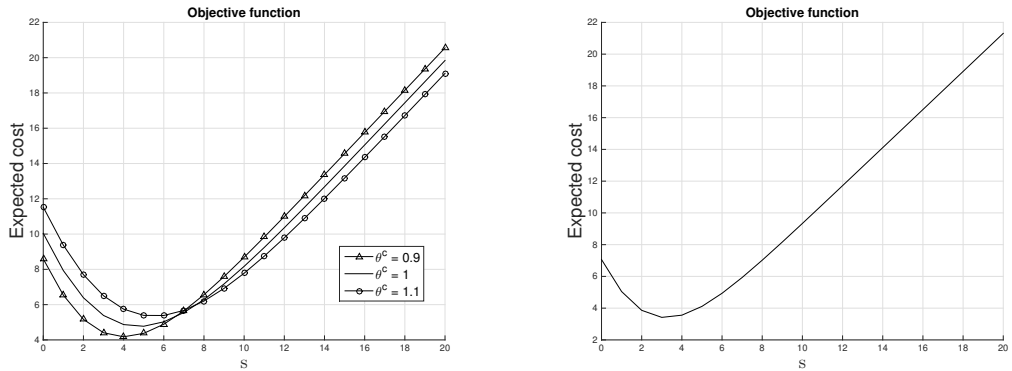
$$c_t := c_H(R_{t-1} + I_t^+) + c_B I_t^-,$$

where  $a^- := -\min\{a, 0\}$ . The expected total cost over  $\mathcal{T}$  period is therefore

$$H_s(\theta^c) := \mathbb{E}[h_s(\xi)] = \mathbb{E} \left( \sum_{t=1}^{\mathcal{T}} c_t \right),$$

where  $\xi = [\mathcal{D}_1, \mathcal{D}_2, \dots, \mathcal{D}_{\mathcal{T}}]^\top$  and  $h_s(\cdot)$  denotes the objective function corresponding to the order-up-to level  $s$ . In all of our experiments, we set the parameters as  $c = 0.5$ ,  $c_H = 0.1$ ,  $c_B = 0.2$  and  $\mathcal{T} = 12$ , where each period represents a month. Two cases will be investigated.

- (i) **Single source of IU:** the demands are assumed to be i.i.d. exponential r.v.s with mean  $\theta^c = 1$ .
- (ii) **Multiple sources of IU:** the demands are independent exponential r.v.s, but the means for each quarter are  $\theta^c = [1, 0.8, 0.5, 0.5]^\top$ .



(a) Single source of IU: perturbing  $\theta^c$ .

(b) Multiple sources of IU:  $\theta^c = (1, 0.8, 0.5, 0.5)$ .

Figure 4.2: Production-inventory problem: true objective functions.

We will consider selecting the best design among  $s = \{1, 2, \dots, 20\}$ . The objective



functions for both cases are plotted in Figure 4.2, where Figure 4.2 (a) shows how sensitive the best design is to IU in case (i). Notice that the best design under the true parameter  $\theta^c$  is 5, but it gets perturbed into designs 4 and 6 for  $\theta^c = 0.9$  and  $\theta^c = 1.1$ , respectively. In Figure 4.2 (b), design 3 is the best one. In addition, in case (i), the likelihood ratio for  $\nabla H_i(\theta)$  is

$$\frac{\nabla_{\theta} f(\xi; \theta)}{f(\xi; \theta)} = \frac{\sum_{t=1}^T \mathcal{D}_t - T\theta}{\theta^2}.$$

Similarly, the likelihood ratio for  $\partial H(\theta)/\partial \theta(q)$  in case (ii) is

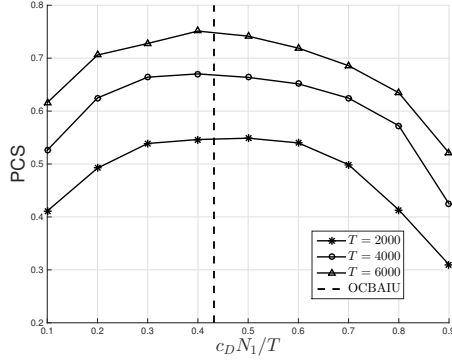
$$\frac{\partial H(\theta)}{\partial \theta(q)} = \frac{\sum_{t=3q-2}^{3q} \mathcal{D}_t - 3\theta(q)}{[\theta(q)]^2}, \quad 1 \leq q \leq 4.$$

Also, we have  $\Sigma_{\theta}(q) = [\theta(q)]^2$  and  $\Sigma_{\theta^c} = \text{diag}([\theta^c(1)]^2, [\theta^c(2)]^2, [\theta^c(3)]^2, [\theta^c(4)]^2)$ , where “diag” denotes a diagonal matrix.

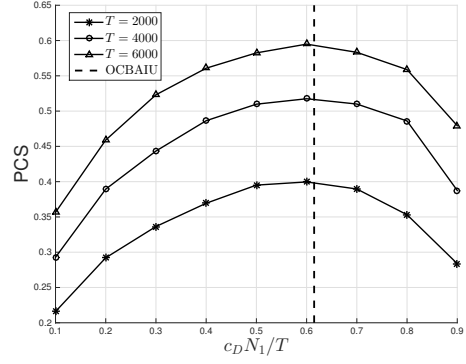
#### 4.4.2 Results for OCBAIU

**Single source of IU.** We test OCBAIU on two cost configurations:  $c_D = 2, c_S = 1$  and  $c_D = 10, c_S = 1$ . First, we use (4.3.7) to compute  $c_D N_1/T$ , i.e., the fraction of budget allocated to data collection, and compare it with the optimal fractions under  $T = 2,000, 4,000, 6,000$ . To find out the optimal fraction empirically, we let  $c_D N_1/T$  take values on a grid  $0.1, 0.2, \dots, 0.9$  and use OCBA in the second stage. When implementing OCBA, we use 20% of the simulation budget for initial estimation, and the budget increment per iteration is 20. The results are shown in Figure 4.3, where the dashed line is the fraction computed by OCBAIU using the true values of  $\delta_{ij}(\theta^c), \sigma_i^2(\theta^c)$ , etc. It can be seen that OCBAIU’s fraction achieves near-optimal PCS for both configurations of cost parameters.

Next, we examine the performance of OCBAIU when plug-in estimates of  $\delta_{ij}(\theta^c), \sigma_i^2(\theta^c)$ , etc. are used to solve for the optimal N. In doing so, we collect  $N_0 = 20 + 0.002 \times (T -$



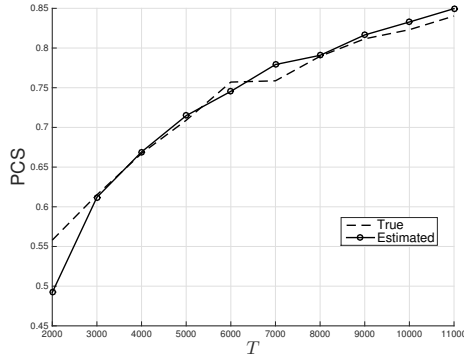
(a)  $c_D = 2, c_S = 1$ .



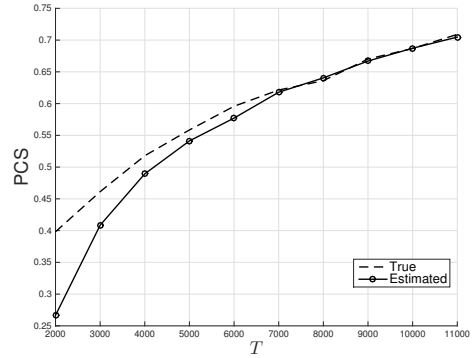
(b)  $c_D = 10, c_S = 1$ .

Figure 4.3: Fraction of budget allocated to data collection computed using true values.

2000) data samples to obtain  $\hat{\theta}_{N_0}$ , and then run  $N_0$  replications for each design using CRN to obtain initial estimates of  $\delta_{ij}(\theta^c)$ ,  $\sigma_i^2(\theta^c)$  etc. In particular, the simulation outputs are reused as initial estimates for OCBA. Figure 4.4 compares the PCS of using true and estimated parameters under growing budget. It can be seen that although estimation error lowers PCS for  $T$  small, the gap diminishes quickly as  $T$  gets larger.



(a)  $c_D = 2, c_S = 1$ .



(b)  $c_D = 10, c_S = 1$ .

Figure 4.4: Single source of IU: PCS curves for OCBAIU using true and estimated parameters.

**Multiple sources of IU.** When there are four independent sources of IU, we also consider two cost configurations:  $c_D = [2, 2, 3, 3]^T$  and  $c_D = [10, 10, 2, 2]^T$  ( $c_S$  is always set to 1 for simplicity). We cannot visualize the empirical optimal fractions in a 4-d space, so

instead the fractions computed by OCBAIU (using true parameters) are shown in Figure 4.5. One can see that, as data for the last two quarters become cheaper compared with the first two quarters, OCBAIU effectively recommends collecting more data for the third and fourth input distributions. The comparison of PCS between using the true and estimated parameters is displayed in Figure 4.6, where similar observations can be made about the gap between them.

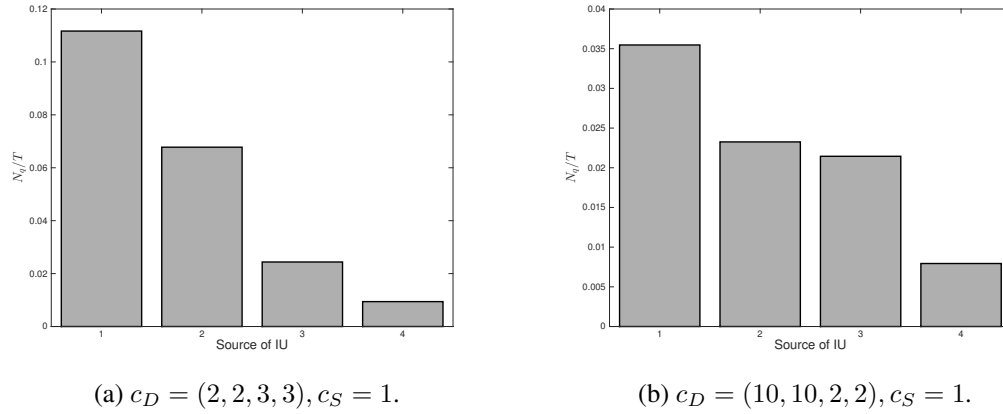


Figure 4.5: Multiple sources of IU: fractions computed by OCBAIU.

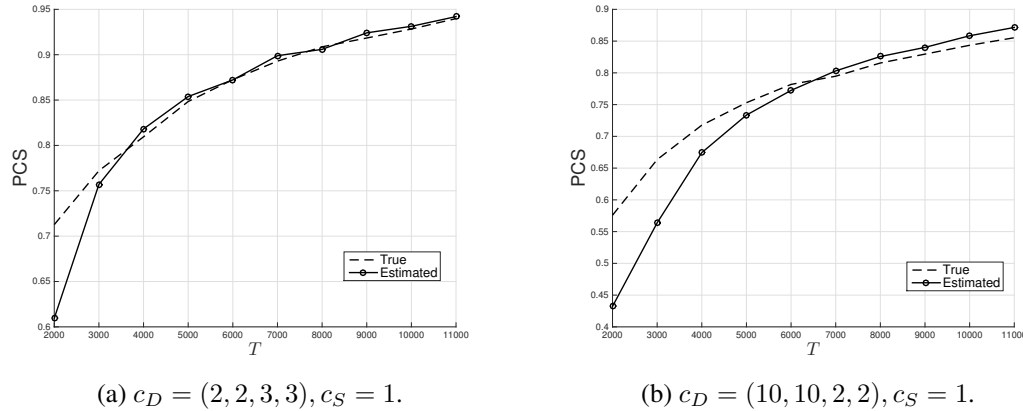


Figure 4.6: Multiple sources of IU: PCS curves for OCBAIU using true and estimated parameters.

Based on the above results, we conclude that OCBAIU is able to adapt to different configurations of IU and cost parameters, and achieve a near-optimal PCS even if the unknown

parameters are subject to estimation error.

#### 4.4.3 Results for Fixed Confidence Algorithms

We test SE-IU, Pairwise SE-IU and the heuristic algorithm in the same settings of single and multiple sources of IU. Specifically, we run these algorithms under batches of input data and simulation outputs. The batch sizes per stage are 100, 1,000 and 10,000. For example, if the batch size is 100, then at each stage we collect a batch of 100 additional data samples for each input distribution, and average each batch into a single aggregated sample; similarly, 100 additional replications are run for each design, and the simulation outputs are aggregated into a single output through averaging. The different batching schemes help us test our algorithms under different degrees of IU and SU.

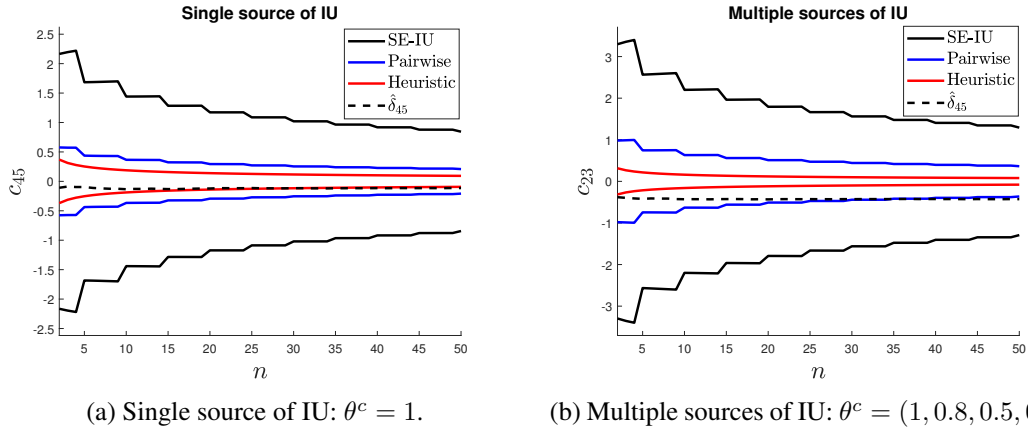


Figure 4.7: Continuation regions.

In all our experiments, we set  $\eta = 0.2$  for the moving average estimators, i.e., the first 20% of the simulation outputs are discarded. For an intuitive comparison, we plot out some realizations of the three algorithms' confidence bounds  $\{c_{45,n}\}$  and  $\{c_{23,n}\}$  under batch size 1,000 in Figure 4.7. It can be seen that our pairwise Sequential Elimination framework indeed leads to smaller continuation regions. The dashed lines in Figure 4.7 (a) and (b) are the trajectories of  $\hat{\delta}_{45,n}$  and  $\hat{\delta}_{23,n}$ , respectively. On these illustrative sample paths, the heuristic algorithm is the fastest one to eliminate the inferior designs (i.e., designs 4 and 2).

In particular, in Figure 4.7 (b), it is able to eliminate design 2 right from the first stage. In contrast, the other two algorithms need more stages to distinguish between the designs.

Table 4.4.1: Expected number of stages used by different algorithms.

| Batch size<br>per stage | Single source of IU    |          |           |
|-------------------------|------------------------|----------|-----------|
|                         | SE-IU                  | Pairwise | Heuristic |
| 100                     | $\geq 10,000$          | 3,451    | 593       |
| 1,000                   | $\geq 5,000$           | 302      | 49        |
| 10,000                  | 606                    | 19       | 3         |
| Batch size<br>per stage | Multiple sources of IU |          |           |
|                         | SE-IU                  | Pairwise | Heuristic |
| 100                     | $\geq 10,000$          | 4,279    | 156       |
| 1,000                   | 3,384                  | 335      | 11        |
| 10,000                  | 161                    | 20       | 1         |

Next, we estimate the expected running time (in terms of stages) for different batch sizes using 1,000 independent replications. We set  $n_0 = 1$  for SE-IU and Pairwise SE-IU. The results are summarized in Table 4.4.1, where the PCS for all the experiments are close to 1 and thus is omitted. Clearly, SE-IU is too conservative and it has impractical running times on this problem instance. Pairwise SE-IU has a more reasonable running time, but the heuristic algorithm has much higher efficiency. Notably, under batch size 10,000, the heuristic algorithm only takes on average one stage to terminate. In that case, the IU and SU are sufficiently low and the confidence bounds reduce to simultaneous confidence intervals. This means that Pairwise SE-IU can be useful even if no further data can be collected, as it can serve as a tool for checking whether the existing simulation outputs let us confidently select the best design.

## 4.5 Conclusion and Future Work

We study Ranking and Selection under input uncertainty in cases where additional data can be collected. Two classical formulations, fixed confidence and fixed budget, are extended

to the new settings. For fixed confidence, we extend and modify a Sequential Elimination framework to allow pairwise comparisons, which leads to algorithms that are more efficient than a direct extension of Sequential Elimination. For fixed budget, we propose the OCBAIU algorithm, which achieves near-optimal PCS by balancing input uncertainty and simulation uncertainty. Numerical results demonstrate the effectiveness of our algorithms. Overall speaking, our fixed confidence algorithms tend to overshoot the PCS target. Our future plan is to explore other methods to construct tighter confidence bounds so that the efficiency can be further enhanced. Another direction is to consider input data that are correlated over time, which exist in many applications such as wind pattern prediction.

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